University of Alberta

Extending diluent limits in methane/air combustion by adding simulated reformer gases

by

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Curse, bless, me now with your fierce tears, I pray.
Do not go gentle into that good night
Rage, rage against the dying of the light.

Dylan Thomas

Life is intrinsically, well, boring and dangerous at the same time. At any given moment the floor may open up. Of course, it almost never does; that's what makes it so boring.

Edward Gorey

To those who have written to the age-old brotherhood of Rosicrucians for a free copy of their book 'The Mastery of Life' in order to release the inner consciousness and to experience (in the privacy of the home) momentary flights of the soul

ABSTRACT

The laminar burning velocities (S_u) of methane (CH_4)-air, CH_4-air-diluent and CH_4-air-diluent-reformer gas ($CO + H_2$) mixtures have been measured using a constant volume cubical combustion chamber. The burning velocities have been measured from the pressure rise inside a cubical combustion chamber with the help of a multi-zone thermodynamic equilibrium model. The initial pressure was always maintained at either 1 atm or 2 atm. The gases were mixed in proper proportion using the method of partial pressures. A mixture containing 81.5% N_2 and 18.5% CO_2 was used to simulate the exhaust gases. The mixture was chosen by matching its specific heat capacity with that of the products of combustion of stoichiometric CH_4-air combustion. The S_u of the stoichiometric CH_4-air mixture was found to be 34.9 cm/s. The S_u gradually decreased as simulated exhaust gas was added to the mixture. The variation of volumetric percentage of reformer gas-air required to raise the S_u back to undiluted levels was measured. The S_u of hydrogen-carbon monoxide-air over a range of hydrogen and carbon monoxide volume fractions were also measured.

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NOMENCLATURE

S_u ..... Laminar Burning Velocity

C_P ..... Specific Heat at Constant Pressure

C_V ..... Specific Heat at Constant Volume

r_c ..... Compression Ratio

ν ..... Specific Heat ratio (C_P/C_V)

ν_u ..... Specific Heat ratio of Unburned Gases

η_{th} ..... Thermal Efficiency

t ..... Time

mf ..... Mass Fraction

mf_b ..... Burned Mass Fraction

mf_u ..... Unburned Mass Fraction

P ..... Pressure at any instant, t

P_i ..... Initial Pressure before Combustion

P_e ..... Pressure after Combustion

P_{el} ..... Equilibrium Peak Pressure from Stanjan

T ..... Temperature

T_u	Unburned Gas Temperature
T_b	Burned Gas Temperature
ϕ	Equivalence Ratio
EG	Exhaust Gas
SEG	Simulated Exhaust Gas
EGR	Exhaust Gas Recirculation
NGV	Natural Gas Vehicles
RG	Stoichiometric mix of Reformer Gas-Air
DAQ	Data Acquisition
MTEM	Multi-Zone Thermodynamic Equilibrium Model
$\mathcal{V}_H$	Percentage Hydrogen by Volume
$\mathcal{V}_{CO}$	Percentage Carbon monoxide by Volume
$\mathcal{V}_A$	Percentage Air by Volume
$\mathcal{V}_{SEG}$	Percentage SEG by Volume
$\mathcal{V}_{RG}$	Percentage RG by Volume

CHAPTER 1

Introduction

The problems of air pollution and global warming have led to an interest in using alternative fuels. Methane (CH_4) is being used as fuel for internal combustion (I.C) engines through out the world. In this study the effect of simulated exhaust gas (SEG) addition to the laminar burning velocity (S_u) of CH_4-air combustion is investigated.

S_u is one of the most fundamental properties of any air-fuel mixture. It is defined as the velocity of the flame wave with respect to unburned gases [1]. S_u is a function of pressure, temperature and mixture composition and is the most important parameter in the prediction of the performance and safety of combustion devices. It is also one of the most significant input parameters in combustion models. Barnard and Griffiths [2] referred to it as one of the basic measurements of the premixed flame, an accurate knowledge of which is important in any combustion study, so the knowledge of S_u is of paramount importance for our understanding of fundamental combustion processes and for direct practical applications aimed at increasing the fuel ef-

ficiency and reducing pollutant emissions from combustion devices in general.

The use of alternative fuels such as hydrogen (H_2), CH_4, methanol and ethanol makes knowledge of S_u of these fuels of paramount importance. Lean CH_4-air combustion and stoichiometric CH_4-air combustion with exhaust gas recirculation (EGR) are receiving attention due to the fact that they ensure complete burning and produce less pollution due to lower emission of the oxides of nitrogen [3,4,5,6]. The EGR in particular is a very useful technique at higher load conditions where NO_X emissions are at their peak as EGR lowers flame temperature and peak pressure.

The most commonly used operating cycle for I.C. engines is the Otto cycle. The thermal efficiency of an ideal Otto cycle can be expressed in terms of compression ratio and specific heat ratio as follows:

$$\eta_{th} = 1 - \frac{1}{r_c^{(\nu-1)}} \tag{1.1}$$

When EGR is used in an I.C. engine running on Otto cycle, it permits use of higher compression ratios, which in turn improves the thermal efficiency of the engine to a greater extent.

As well as the advantages mentioned above, EG addition has its drawbacks. It leads to a decrease in the S_u of the mixture which results in increased heat

loss, poor combustion phasing and misfiring, which in turn lead to lower fuel efficiency. To reverse the effects of a lower S_u and to prevent all the above mentioned negative effects, a fuel mixture with a higher S_u can be added to the CH_4-air-EG mixture. The blending fuel is reformer gas (75 % H_2 and 25 % CO, the same composition obtained by steam reforming of CH_4). The purpose of adding this mixture is to reap the benefits of EGR and at the same time preventing lower S_u from affecting the performance of combustion systems while also limiting the peak temperature which results in less NO_X emissions. In previous studies it has been found that adding H_2 to a lean fuel-air mixture can resolve combustion stability problems while retaining lower combustion temperatures, which results in lower production of oxides of nitrogen. Allenby et al. [7] showed that when H_2 supplementation was employed, significant gains could be attained in terms of exhaust emissions without the rapid reduction in combustion stability typically seen when applying EGR to a CH_4-fuelled engine. Now, efficient production of H_2 to use in such cases might not be an easy process to deal with. The steam reforming of CH_4 is being used more and more for this purpose in stationary combustion systems, such as gas turbines. Predicting the accurate amount of RG required to raise the S_u of the mixture back to the undiluted level must be done experimentally. Therein lies the need to perform rigorous testing to raise the S_u of the CH_4-air-EG mixture back to the stoichiometric CH_4-air level.

In this study the laminar burning velocities of CH_4-air-simulated exhaust gas (SEG), CH_4-air-SEG-reformer gas (RG) mixtures have been measured us-

ing a constant volume combustion chamber. The burning velocities have been measured from the pressure rise inside a cubical combustion chamber with the help of a multi-zone thermodynamic equilibrium model. The effect of diluents on methane-air burning velocity and the amount of reformer gases required to restore the undiluted burning velocity are also measured.

In Chapter 2, a detailed review of previous literature on the burning velocity of stoichiometric CH_4-air mixtures, CH_4-air-diluent mixtures is given. A review of studies on EGR and hydrogen supplementation in S.I. engines was also done. In addition to that the reasons for choosing methane as the fuel, using hydrogen as a supplement and employing the constant volume method are provided.

Chapter 3 provides a detailed account of the combustion chamber, the ignition system, the gas mixing system, the pressure and temperature transducers and the data acquisition system that was used in the experiments. Description of the experimental set up and explanation of the experimental procedure are also given. Chapter 4 is a paper titled "Maintaining burning velocity of exhaust-diluted methane-air flames by partial fuel reformation" which was accepted at the Combustion Institute Canadian Section Spring Technical Meeting in 2004 and has been submitted to the International Flame Research Foundation Journal. The burning velocities measurements of stoichiometric methane-air, methane-air-exhaust and methane-air-exhaust-reformer gas mixtures are given.

Chapter 5 is a paper titled "Burning velocities of laminar premixed Carbon monoxide-Hydrogen/Air mixtures" which is under preparation to be submitted to the Journal of Automobile Engineering. This study presents the burning velocities of hydrogen-carbon monoxide-air mixtures over a range of H_2 and CO volume fractions. Chapter 6 provides a summary of the conclusions arrived at in these two studies, the recommendations and the direction of future work at the University in this area.

CHAPTER 2

Literature Review

In this chapter thorough details of works done on methane (CH_4)-air burning velocities, CH_4-air-diluent burning velocities and hydrogen (H_2) supplementation of fuel-air mixtures are presented.

2.1 Why Methane?

The reasons for choosing CH_4 as a fuel is because it is being used as a fuel for I.C. engines throughout the world, especially in Canada which is the world's third largest producer of natural gas (over 90 % of the production is from Alberta [8]). Figure 2.1 [9] shows the population of Natural Gas Vehicles (NGV) in Canada and in Argentina from 1984 to 2003. From the latest census done in 2003 we can infer that NGVs are on the increase throughout the world from developed countries to developing countries. Argentina has almost 10 million NGVs and Canada has about 25000 NGVs presently, and they have been on the increase ever since they have been introduced in both the countries. These two countries gives us both ends of the spectrum, since

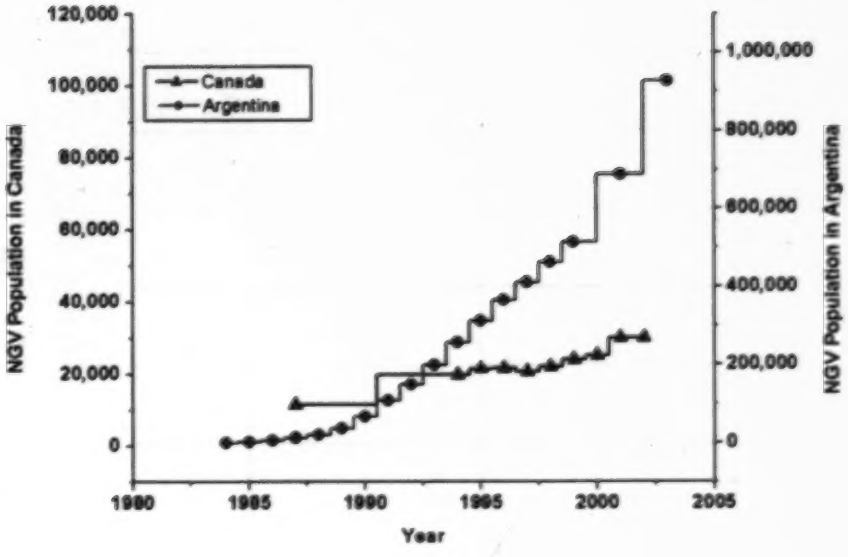


Figure 2.1: Natural Gas Vehicle (NGV) Population for Argentina and Canada (Note different y-axes)

Canada is rich in its oil and petroleum products and Argentina relies on imports for all of its oil and petroleum products.

Natural gas engines generally show very low emissions of reactive hydrocarbons, carbon monoxide, and particulate matter. NO_X emissions can be fairly high [10], but this can be eliminated by using EGR.

2.2 Why Hydrogen?

The S_u of CH_4-air mixtures is low when compared to gasoline-air, so using H_2 as a supplement to CH_4-air mixtures and CH_4-air diluent mixtures has its merits. There are several advantages of using H_2 as a supplement to the regular fuel in a S.I. engine running on a lean CH_4-air mixture or CH_4-air mixture along with diluents from EGR. The following are some of the them:

- H_2 can sustain vigorous burning even under lean conditions and low temperatures when compared to most other hydrocarbons.
- The S_u of H_2 is relatively high (240 cm/s) when compared to that of CH_4 (35 cm/s). This allows the use of higher percentages of EG without having a negative effect on the efficiency of the engine due to slower combustion.
- H_2 does not contain any carbon, so it eliminates the direct emissions of carbon compounds from the fuel that it replaces.
- H_2 supplementation helps in the reduction of the emission of oxides of nitrogen if the engine can be operated with a high percentage of EGR.
- The addition of H_2 to CH_4-air diluents overcomes flame initiation and flame propagation problems associated with CH_4-air combustion. [11]

2.3 Why Reformer Gas?

The next big question in using H_2 to increase the S_u of the EGR diluted fuel mixture back to that of stoichiometric levels, is the production of H_2 to be used in such cases. Finding an efficient way to produce H_2 to be used in such cases remains a huge technological challenge. Some of the methods of production of H_2 are steam reforming of CH_4, partial oxidation, coal gasification, electrolysis and thermochemical decomposition. The most economically efficient way is by steam reforming of CH_4 [12]. Approximately 96 % of the H_2 produced in the world is by some form of steam reforming of carbonaceous fuel. The next challenge is the storage of H_2 in an automobile. H_2 can be stored as a metal hydride or as a cryogenic liquid or in gaseous form. Each method of storage has its own disadvantages. When stored as a hydride, the fuel system weight becomes a huge drawback. When stored as a liquid, the volume it occupies is very high and liquefaction is expensive. When stored as a gaseous form, the weight and safety of high pressure tanks become issues.

In light of the various drawbacks associated with the storage of H_2, on-board production of H_2 could be looked at very closely. On board reforming of fuels to produce reformer gases (RG - CO-H_2 mixture) in such cases is in initial stages of development to be used in commercial vehicles [13]. It is already being used in stationary engines, and turbines [14] where EGR is employed. There are two methods for on-board reforming using the CH_4 already available in the vehicle, either by partial oxidation of CH_4 or by steam reforming. Partial oxidation is an exothermic process and the heat energy produced as a result might be an unnecessary problem, but on the other hand steam

reforming of CH_4 is an endothermic process, so the wasted heat from the exhaust gases can be cultivated for this purpose.

In all the above mentioned cases of H_2 production, the byproduct obtained is CO. The CO obtained can be removed by water-gas shift reactions and then H_2 recovery. These processing steps add a significant cost to H_2 production. In the case of S.I. engines, RG can be used directly to increase the S_u after EGR addition without removing the CO, as it simply increases the available energy in the fuel. Hence, for RG simulation in the experiments, the same volume percentage of the products obtained from the steam reforming of CH_4 is used.

2.4 Why Constant Volume Method?

Over the course of several years many different methods have been developed to calculate burning velocities of premixed gaseous fuels. Some of them are conical flames, adiabatic counter flow burners, constant pressure techniques, and the constant-volume combustion bomb. Different methods of measuring burning velocities have been critically reviewed by Andrews and Bradley [15], Linnett [16] and Rallis and Garforth [17].

Andrews and Bradley [15] did a review of all the methods and experimental techniques used for the measurement of burning velocities. They concluded that there was no standardized method of measurement. They classified the experimental techniques into two broad divisions:

- Non Stationary flames and
- Stationary flames.

Some of the Non Stationary flame techniques they reviewed were: Tube method: It involves igniting the mixture at the open end of the tube and photographing the flame front propagation towards the closed end. Contained Explosions: In this case there is a containing envelope surrounding the fuel-air mixture, with a central ignition usually. Then the rate of propagation of the flame front is measured. There are different methods of calculating the burning velocity using contained explosions technique. There are various methods in the stationary flame technique to measure the burning velocity, the most popular one being the nozzle method and the burner method. The authors finally concluded that the closed vessel explosion technique as used in this study has good possibilities for the accurate measurement of burning velocity.

The constant volume method has been described by Linnett [16] as a potentially powerful method for determining burning velocities. Rallis and Garforth [17] stated that if the full potentialities of the constant volume method were used, it can yield considerably more information from a single experiment than can any other method.

The present study uses a constant volume cubical combustion chamber to measure the burning velocities of fuel-air mixtures. The main advantages of

using a constant volume combustion bomb are listed below:

- It facilitates the determination of burning velocity over a range of pressure and temperature.
- It facilitates high speed photography.
- Premixing can be achieved relatively easy.
- Burning velocity can be obtained from a single pressure trace with the initial temperature and pressure.

2.5 Burning Velocities of Methane-Air Mixtures

Iijima and Takeno [18] investigated the effect of temperature and pressure on the burning velocity of CH_4-air mixtures using the spherical bomb technique. They covered equivalence ratios from 0.8 to 1.3 and varied the mixture temperature from 291 to 500 K. The pressure was varied from 0.5 to 30 atm. The measured stoichiometric CH_4-air S_u was 35 cm/s at an initial pressure of 1 atm and initial temperature of 291 K. They also did a comparison of the on the burning velocities obtained by different methods and noticed that the S_u obtained by the constant volume method agree well with each other and was always lower compared to the other methods, but they did not reach any conclusion on the reason for that discrepancy.

Clark et al [19] measured the S_u of CH_4-air at different equivalence ratios within a constant-volume combustion bomb in a micro-gravity environment.

The micro-gravity method eliminated the buoyancy effects and enables measuring the S_u in a large range of pressure from a single experiment. They covered equivalence ratios from 0.6 to 1.4 and used the Lewis and von Elbe model to calculate the S_u. They found the stoichiometric CH_4-air S_u to be 35.4 cm/s at an initial condition if 1 bar and 298 K.

Hassan et al [20] measured the S_u of CH_4-air mixtures at condition of equivalence ratios of 0.6 to 1.35, initial pressures of 0.5 to 4 atm and initial temperature of 298 K. They used a spherical constant volume combustion chamber for their experiments. They also investigated the effect of stretch on the S_u both experimental and computationally. They found the stoichiometric CH_4-air S_u to be 35 cm/s at 1 atm and 298 K.

Agarwal [21] investigated the S_u of CH_4-air mixtures at various initial mixture compositions and pressures. A spherical constant volume combustion vessel was used for the experiments. He covered equivalence ratios from 0.8 to 1.2 and varied the initial pressure from 0.4 to 10 atm and found that the S_u is dependent on the reciprocal of the pressure. The stoichiometric CH_4-air S_u was found to be 34 cm/s at 1 atm and 298 K. From these four studies, the mean S_u obtained is 34.85 cm/s with $\sigma = 0.6$ cm/s.

The following are the burning velocities obtained from using methods other than constant volume. Generally it can be noticed that the burning velocities obtained are higher relative to the constant volume. It is speculated that it might be because of the feed back of heat in the burner methods, whereas in

the constant volume bomb there is no feedback of heat. The stoichiometric CH_4-air burning velocities obtained from studies done by Bosschaart et al (Heat Flux Burner Method: 36 cm/s) [22], Egolfopoulos et al. (Counter Flow Flames: 39 cm/s) [23], Gunther and Janisch (Burner Method: 40 cm/s) [24], prove that burning velocities obtained from constant volume method is generally lower. It can also be concluded from the values of the stoichiometric CH_4-air burning velocities from the above mentioned studies [18, 19, 20, 21] that the data obtained from studies done using the constant volume method agree well with each other and the variation is lower compared to the studies done by other methods. The stoichiometric CH_4-air laminar burning velocities from these previous studies are used as a datum to compare the S_u of stoichiometric CH_4-air combustion obtained in this study.

2.6 Burning Velocities of Methane-Air-Diluent Mixtures

Although there is a significant amount of literature pertaining to the S_u of CH_4-air, there is far less for CH_4-air-diluent mixtures. Ryan and Lestz [25] used a constant volume bomb to determine the basic combustion characteristics including the S_u of air-fuel mixtures in the presence of a diluent at different unburned gas temperatures. They also used a thermo-chemical kinetic model to predict the concentrations of nitric oxide during combustion and in the burned gas. Wierzba et al. [26] investigated the rich and lean flammability limits of fuel containing diluents. The effect of temperature

was also investigated. Clarke et al. [19] measure the S_u of CH_4-air mixtures at different equivalence ratios with various levels of carbon dioxide, nitrogen or a mixture of these two as diluents. They also studied the S_u of biogas (CH_4 with 35 % carbon dioxide) using a spherical constant-volume combustion vessel. They used the Lewis and vol Elbe method [1] to calculate the S_u. They went as high as 20 % diluents and 80 % CH_4-air and at this volume percentage the S_u was not consistent.

Stone and Clarke [27] studied the S_u of CH_4-air-diluent mixtures for variations in unburned gas temperature from 293 K to 454 K and pressures from 0.5 bar to 10.4 bar. Again they used a spherical constant volume vessel in microgravity environment and the Lewis and vol Elbe method [1] to calculate the S_u. The correlations of S_u reported by them were for CH_4-air-diluent mixtures, in which the diluent mixtures were varied from carbon dioxide or nitrogen or a mixture of these two. They covered a higher level of diluent than previously reported for either nitrogen or carbon dioxide. The effect of SEG on the burning velocity of the methane-air mixture was 1.2 $\frac{cm/s}{\%_{SEG}}$.

Elia et al. [28] used a spherical constant volume combustion cell again to calculate the S_u of CH_4-air diluent mixtures. The used diluent concentrations as high as 15 %. They developed a correlation for a range of pressures from 0.75 atm to 70 atm, unburned gas temperatures from 298 K to 550 K, equivalence ratios from 0.8-1.2 and diluent addition from 0-15 % by volume. The effect of SEG on the burning velocity of the methane-air mixture was 1.7 $\frac{cm/s}{\%_{SEG}}$.

The S_u data from these previous studies are used to compare the S_u data of CH_4-air-diluent mixtures obtained in this study. In short although there is a significant amount of literature pertaining to the S_u of CH_4-air there has been little work done on CH_4-air-EG and CH_4-air-EG-RG mixtures. In this study the diluents have been varied from 0-22 % at 1 atm initial pressure and upto 30 % by volume at 2 atm initial pressure.

2.7 Effect of Exhaust Gas Recirculation (EGR)

Quader [29] investigated the effect of intake charge dilution by exhaust gas addition in S.I. Engines. He concluded that NO emissions dropped as the peak in-cylinder temperatures decreases and the specific heat of the reactants increase as a direct result of the exhaust gas addition. Abd-Alla [30] did an extensive review of the use of EGR in I.C. engines and concluded that the use of EGR is most effective in improving exhaust emissions. Quader et al. [13] investigated the use of RG to operate an engine under very lean condition or heavy EGR concentrations. They found that NO_X emissions dropped down considerably. Abd-Alla et al. [31] studied the effects of exhaust gas recirculation (EGR) on combustion and emissions in an indirect injection dual fuel engine. They found that the admission of diluents resulted in reductions in the exhaust NO_X emissions. It can be inferred from these previous studies that EGR plays an important role in decreasing the exhaust emissions.

2.8 Effect of Hydrogen Addition

Brasheas et al. [32] investigated the effects of partial H_2 injection in an I.C. Engine to allow burning of gasoline at ultra-lean conditions. They investigated the emissions and fuel economy. The required H_2 is produced onboard in the generator. Houseman and Hoehn [33] presented the first engine dynamometer test results for a modified fuel system based on H_2 enrichment for a V-8 I.C. engine. The engine burns mixtures of gasoline and H_2 under ultra-lean conditions to yield extremely low NO_X emissions with increased engine efficiency. The H_2 for use was produced in a compact onboard generator from gasoline and air. Stebar and Parks [34] modified a passenger car to operate at 0.55-0.65 equivalence ratio with supplemental H_2. Even though NO_X emissions dropped down considerably, the hydrocarbon emissions increased markedly at these lean conditions.

Kukkonen [12] investigated the feasibility of using H_2 as a replacement in I.C. Engines and compared it with synthetic fuel/vehicle options and with battery-powered EV's. Nagalingam et al. [35] compared the performance of an AVL research engine running on natural gas, H_2 supplemented natural gas and H_2. They investigated engine performance, fuel economy and emissions. Swain et al. [11] investigated the effects of H_2 addition on natural gas engine operation. They concluded that H_2 supplementation reduces both flame initiation and flame propagation problem and that the engine can run lean without increasing the ignition delay or combustion duration.

Jamal and Wyszynski [36] reviewed the use of H_2 and H_2-enriched gaso-

line as a fuel for S.I. engines and the techniques used to generate H_2 from liquid fuels such as gasoline and methanol, on-board the vehicle. They concluded that the use of reformed fuel in Spark Ignition engine might result in lower exhaust emissions. Andreatta and Dibble [37] studied the use of use of air-reformed natural gas (natural gas broken down into H_2 and carbon monoxide) in a spark-ignition engine. They concluded that the H_2 in the reformed fuel allowed the engine to run leaner than when running on natural gas. At the leaner equivalence ratios low levels of NO_X were observed. Carbon monoxide and hydrocarbons were generally reduced by the reformed fuel.

Allenby et al. [7] showed that when H_2 supplementation was employed, significant gains can be attained in terms of exhaust emissions without the rapid reduction in combustion stability typically seen when applying EGR to a CH_4-fuelled engine. Sung et al. [38] studied the effects of RG addition on the S_u of mixtures of n-butane and iso-butane. Their objective was to computationally explore the feasibility of extending the dilution limit of an engine during cold-start conditions by adding RG and to enhance both the ignitability and flammability.

It can be shown from these previous studies that H_2 supplementation of the fuel is possible and had positive effects on the engine efficiency and decreases the emission of NO_X, carbon monoxide and hydrocarbons. It also helps reduce the flame initiation and flame propagation problems. There is no data on the restoration of methane-air-diluent burning velocities.

2.9 Burning Velocity of Carbon Monoxide-Hydrogen-Air Mixtures

Scholte et al. [39] studied the S_u of pure carbon monoxide, carbon monoxide mixed with trace amounts of H_2, carbon monoxide with water vapour and carbon monoxide with CH_4 and propane. The maximum amount of H_2 added was around 4 % by volume. However, all their mixtures were rich, they used 50 % fuel by volume in all their experiments. McLean et al. [40] studied 95 % CO + 5 % H_2 and equimolar mixture of CO-H_2 at different equivalence ratios using a spherical constant volume bomb. Their primary objective was to determine the rate of CO + OH reaction.

Vagelopoulos et al. [40] studied the S_u of very lean mixtures (80 % air) of CO-H_2 at different H_2 mole fractions. They did their experiments using the counterflow, twin flame technique. They concluded that the addition of small quantities of H_2 to CO increases the S_u. Linteris [41] studied the S_u of premixed CO-Ar-O_2-H_2 flames inhibited by CF_3H using the burner method. Brown et al. [42] measured the Markstein lengths of three fuel mixtures: 95 %-5 % CO-H_2, 50 %-50 % CO-H_2 and 100 % H_2. They used a spherical constant volume combustion chamber.

Hassan et al. [43] studied the effects of positive stretch on the S_u in CO-H_2-air mixtures in a constant volume spherical combustion chamber. They went from 3-50 % H_2 in the fuel, equivalence ratios from 0.6-5 and pressures of 0.5-4.0 atm. Rightley et al [44] investigated the S_u of CO-O_2 along with an

inert and trace amounts of H_2 containing species. Their aim was to understand the CO flame structure. Rumminger et al. [45] investigated the S_u of $CO\text{-}H_2\text{-}O_2\text{-}N_2$ with and without iron pentacarbonyl over a range of O_2 and H_2 fractions using the burner method and a schlieren imaging system. They compared the S_u of the inhibited and the uninhibited flames.

In short a varied range of $CO\text{-}H_2$-air mixtures have not been studied by varying the equivalence ratios and also the percentage of H_2 in the $CO\text{-}H_2$-air mixtures. This is the exact objective of the this study.

CHAPTER 3

Experimental Apparatus and Procedure

3.1 Cubical Combustion Chamber

The main apparatus, a constant volume cubical combustion chamber shown in Figure 3.2 consists of a constant volume cubical combustion chamber of edge length 125 mm with a central ignition point [46, 47, 48, 49, 50] (The cubical configuration was developed to allow perforated plate turbulence generation). The chamber is made up of 6066-T6 aluminium alloy. With 25 mm thick walls, the combustion chamber can withstand peak pressures over 1400 kPa allowing initial test conditions around 202 kPa (2 atm). There are also two glass windows mounted on the front and back sides of the combustion chamber to allow optical visualization and photography. The windows are 30 mm thick and 110 mm diameter PK-7 optical glass.

3.2 Ignition System and Spark Electrodes

A capacitive discharge/inductive coil ignition with stored energy of 110 mJ (300 V and 2.5 μf) was used for ignition. A pair of tapered spark electrodes extending from opposite sides of the chamber formed an adjustable gap at the center of the cell. A fixed 3 mm spark gap was used for all tests in this study. It should be noted that the micrometer electrode on one side can be moved relative to the other to obtain different spark gaps. The ignition system is triggered by the Labview program which is also used for data acquisition.

3.3 Test Gas Mixing System

A bottled gas manifold and vacuum pump attached to the system as in Figure 3.3 was used to evacuate the chamber before each run and to meter gas mixtures into the chamber by the method of partial pressures. The methane used in the experiments was 99% pure and dry compressed air obtained from the building was used. The exhaust gases was simulated by a mixture of 81.5% nitrogen (99% pure) and 18.5% carbon dioxide (99% pure). The Reformer Gas was simulated by a mixture of 25% carbon monoxide (99.5% pure) and 75% hydrogen (99% pure). All percentages are composition by volume.

3.4 Pressure and Temperature Transducers

The pressure-time records are obtained using the main pressure transducer which was a flush diaphragm Precise Sensor Model 7820 using a four active arm bonded strain gage. It was calibrated using a dead weight calibrator, and measured pressures from 0 to 1725 $\pm 1\%$ FSO. A Validyne pressure transducer (A) with a range of 0 to 140 ± 0.7 kPa was used to measure cell pressure during filling and was isolated during combustion to safeguard it from high pressures. Another Validyne pressure transducer (B) of the same range was used to measure the pressure in the gas line. This was done to make sure that the pressure in the gas line was always higher than the pressure in the combustion chamber to prevent back flow of gases during filling. A Chromel-Alumel (Type K) thermocouple was used to measure the initial temperatures before each run. The initial temperature were maintained with an accuracy of ± 1°C.

3.5 Data Acquisition System

The data acquisition (DAQ) is performed by a labview program using a on a National Instruments computer interface card (PCI- MIO-16E-4, 12-bit, Pressure resolution of 0.25 kPa) at a sample rate of 5 kHz. The DAQ program sends a 5 Volt pulse to the spark box to produce the spark. It sends another signal to the DAQ card to start recording the pressure from the pressure transducer. All signals are recorded by a DAQ card using a computer and an output excel data file is automatically generated. The output data

file contains information about the initial temperature and pressure of the combustion chamber: fuel, air and diluent and the pressure-time data of the combustion process. A delay was introduced before the signal reaches the spark box so that no data was lost due to the fact that the combustion duration is on the order of a few milli-seconds and a full pressure trace is obtained.

3.6 Procedure

The first step in the experiment is to evacuate the combustion chamber using the vacuum pump. After the combustion chamber has been evacuated, fuel-air-diluent gases are let in one by one into the combustion chamber. Usually the gas with the least partial pressure is let in first. After the first gas with the least partial pressure is let in, the appropriate valves are closed and the gas manifold is evacuated. Then the second gas is let into the combustion chamber. Care must be taken so that the pressure in the gas manifold is always higher than the pressure in the combustion chamber to prevent the back flow of gases in to the gas pipe line. The procedure is repeated over and over until all the gases are filled inside the combustion chamber and the desired initial pressure is achieved. The mixture is allowed to settle down for a few minutes to kill any pre-existing turbulence. The chamber should be evacuated as soon as the combustion finishes to avoid condensation of water before the next run. The accuracy of the mixtures made is dependent on the Validyne pressure transducer used to measure the partial pressures. As explained in Section 3.4 the Validyne is accurate to $\pm 0.5\,\%$ FSO. If a mixture of $10\,\%\,H_2$ is made then it is accurate to $10 \pm 0.5\,\%$. So if for example

a mixture of 10 % H_2 and 90 % air is made, and the partial pressure of H_2 is 100 kPa then it is actually 100 kPa $\pm$ 0.5 %. But at the same time if a mixture of 100 % H_2 is made, then the error will be zero because no other gas is added to the chamber and the chamber has only H_2, so the lesser the number of gases added to the chamber the lower the error due to the Validyne pressure transducer.

3.7 Burning Velocity Calculation

The burning velocity is calculated from the experimental pressure traces using two models: Lewis and von Elbe model and the Multi Zone Thermodynamic Equilibrium Model. These two models are briefly explained in the following sections.

3.7.1 Lewis and von Elbe Model

The burning velocity, unburned mixture temperature, mass fraction burned and the flame radius are calculated by the Lewis and von Elbe method [1] from the time-pressure trace. The procedure is briefly explained below. Say a fraction n of gas before ignition occupies a sphere of volume V_i and radius r_i and after combustion gives rise to a pressure P and if a is the hydraulic radius of the vessel if it were a sphere, T_i the temperature before ignition, T_u is the unburned gas temperature, P_{el} is the equilibrium pressure calculated

from STANJAN [1] [51], and mf_b is the mass fraction burned, then

$$mf_b = \frac{P-P_i}{P_{ei}-P_i} \tag{3.1}$$

$$r_i = a\left(\frac{P-P_i}{P_{ei}-P_i}\right)^{\frac{1}{3}} \tag{3.2}$$

If the volume of the fraction n after burning is V_b and its radius r_b, then

$$r_b = a\left(1 - \frac{P_i}{P}\frac{T_u}{T_i}\frac{P_{ei}-P}{P_{ei}-P_i}\right)^{\frac{1}{3}} \tag{3.3}$$

Now using the two equations given above the burning velocities and the flame speed can be determined. The flame speed can be obtained by finding out the slope of dr_b/dt and the burning velocity is obtained by the equation,

$$S_u = \frac{dr_i}{dt}\left(\frac{r_i}{r_b}\right)^2\left(\frac{P_i}{P}\right)^{\frac{1}{\nu_u}} \tag{3.4}$$

The Lewis and von Elbe model assumes negligible pressure rise and density change so it becomes less accurate for significant pressure rise, therefore the Multi Zone Thermodynamic Equilibrium Model is used.

[1] STANJAN is an interactive program for chemical equilibrium analysis by the method of element potentials. It handles a gas phase and multiple condensed phases. The JANNAF thermochemical tables are used as the primary data base. Each phase is modelled either as a mixture of ideal gases or an ideal solution.

3.7.2 Multi-Zone Thermodynamic Equilibrium Model

A Multi-Zone Thermodynamic Equilibrium Model (MTEM) [49] was used to calculate the unburned mixture temperature, mass fraction burned, flame radius and burning velocity from the pressure trace, mixture composition and initial conditions. The model treats the mass of gas in the combustion chamber as 1500 concentric spherical shell elements. Combustion is modelled by the sequential burning of each element with accompanying expansion of that element, compression of all other elements and consequent pressure rise. The volume of unburned gas burned during each time interval is considered as a thin shell of initial (unburned) radius r_i surrounding the previously burned elements of radius r_{last}, (Figure 3.1). The model calculates the burning velocity using the flame area based on the radius r, which is the geometric mean of r_{last} and r_b, the flame radius after the element burns.

$$r = \sqrt{(r_{last}^2 + r_b^2)/2} \tag{3.5}$$

In this model, each element is considered adiabatic from the adjacent shells. As each of these elements burns, its flame temperature and equilibrium composition are calculated using an iterative scheme which considers only the six principal species ($CO, CO_2, O_2, N_2, H_2, H_2O$) and two principal dissociation reactions, (CO_2 dissociation and the water-gas reaction as represented by the following equations).

$$CO_2 \rightleftharpoons CO + \frac{1}{2} O_2 \tag{3.6}$$

$$CO + H_2O \rightleftharpoons CO_2 + H_2 \tag{3.7}$$

It was shown by Ting [49] that these two dissociation reactions were adequate for the energy analysis of methane-air mixtures. For methane/air combustion at an equivalence ratio of 0.9, the maximum adiabatic flame temperature calculated using STANJAN [51] was 2135 K, while the temperature calculated using MTEM was 2152 K and at an equivalence ratio of 0.7, STANJAN [51] gives a value of 1839 K and MTEM gives a value of 1845 K, which accounts for a variation of less than 1 %.

The chamber shape effects are neglected because the model only focuses on the main stages of flame growth. Thus, the model can only predict the flame growth up until the time the spherical flame touches the walls of the cubical combustion chamber, after which the shape effects of the chamber begin to take control. The flame reaches the wall of the combustion chamber around the time the pressure reaches $2.2\,P_i$, where P_i is the initial pressure. The valid data for the MTEM is then $P_i \leq P \leq 2.2\,P_i$.

The burning velocity is obtained for the entire range of pressure rise. During the initial stages of combustion the fluctuation in the pressure is very high because of the electrical noise due to the spark. Since this might affect the calculation of the actual burning velocity the data from P_i to $1.05\,P_i$ was neglected.

The first step is converting the voltage signal obtained from the pressure transducer into a pressure signal. This is done by the program DATA.m

(Programs are listed in Appendix E). The program BOMB.m calculates the theoretical values of pressure, relative flame radius, mass fraction burnt, temperature of the reactants and temperature of element after combustion from the initial conditions and the percentages of different gases in the mixture. The subroutine EQCONST.m calculates the property coefficients and equilibrium constants, the subroutine EQVALENCE.m calculates the equivalence ratio. Then the subroutine REACTPROP.m calculates various property coefficients for fuel-air mixture. The subroutine fngamR.m calculates the specific heat ratio of the reactant mixtures from constant obtained from EQCONST.m. The program then estimates the pressure after one element burns which is just a guess.

$$P_e = P_i + (Equivalence\ Ratio)\,(P_i)/N_{tot}^{\frac{3}{2}} \tag{3.8}$$

where N_{tot} is the total number of elements, 1500. Then the program calculates the unburned gas temperature and the specific heat ratio of the unburned gases assuming isentropic compression to the the pressure estimate. The unburned gas volume before and after the element burns is then calculated from the pressure estimate and the unburned gas properties. Then the burned gas temperature and volume are calculated at this pressure. Then, an equilibrium calculation and an energy balance is done and the work done by compressing the unburned gases and all previous elements is calculated. If Q is the element heat transfer, U_R is the internal energy of reactants, U_P is the internal energy of the products and W_{Comp} is the work done in compressing the elements, then

$$Q + U_R = U_P + W_{Comp} \tag{3.9}$$

Since the element heat transfer is assumed to be zero and if P_i and V_i are the pressure and volume before the element burns and P_e and V_e are the pressure and volume after the element burns, the work done in compressing the elements is given by

$$W_{Comp} = \Sigma \left[\frac{(P_e V_e - P_i V_i)}{(1-\nu)}\right] \tag{3.10}$$

Then from the work done by the element and starting conditions, the flame temperature is calculated by the subroutine FLAME.m. From the estimated element pressure and the flame temperature obtained from FLAME.m the element volume is calculated. The sum of the element volume and the burned and unburned volume should be equal to the total volume for the pressure estimate to be correct. So the model calculates the flame growth in terms of volume burned, mass burned and pressure rise for a set of initial conditions.

The program BP.m interpolates the results obtained from the theoretical calculations to the experimental pressure trace and calculates relative flame radius, mass fraction burned, temperature of the reactants and temperature of each element after combustion at the experimental pressure. The program BV.m reads the results obtained from BP.m and calculates the flame radius and the burning velocity. The model calculates the burning velocity by using the equation:

$$S_u = dr_i/dt \tag{3.11}$$

All the programs used for calculating the burning velocity are given in Appendix E.

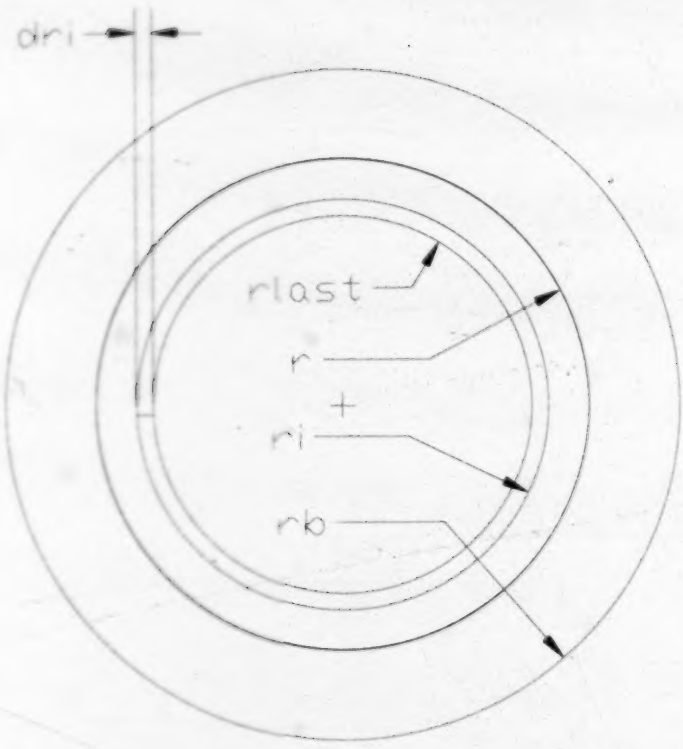


Figure 3.1: Geometric Method used to calculate Burning Velocity

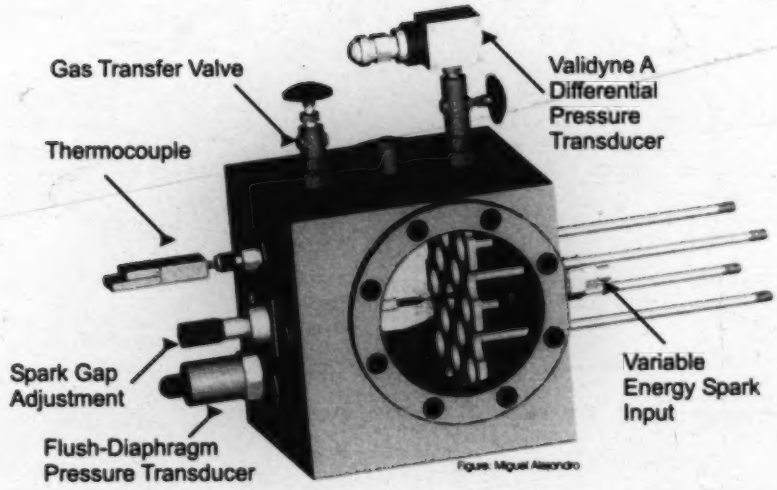


Figure 3.2: The Combustion Chamber

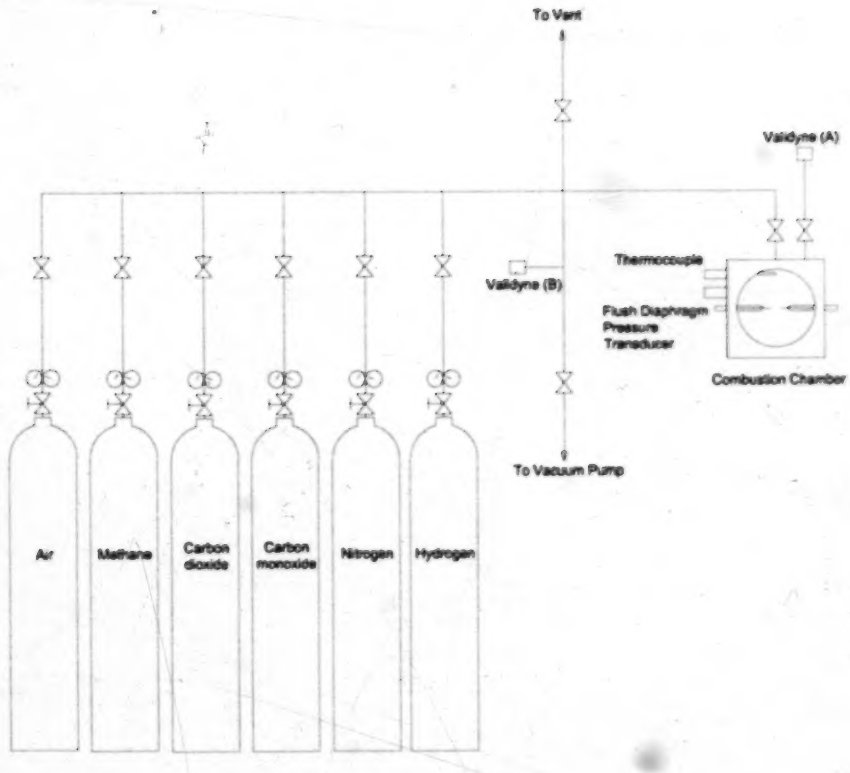


Figure 3.3: Schematic of Gas Filling and Vacuum Manifold

Chapter 4

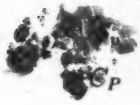
Maintaining burning velocity of exhaust-diluted methane-air flames by partial fuel reformation - CICS 2004 / IFRF Journal, Under Review

4.1 Abstract

The burning velocities of stoichiometric methane-air, methane-air- exhaust and methane-air-exhaust-reformer gas mixtures have been measured using a constant volume cubical combustion chamber. The flame size and burning velocities were calculated from the chamber pressure record using a multi-zone thermodynamic equilibrium model. The investigation measured the decrease in burning velocity due to addition of Simulated Exhaust Gases (SEG) and the quantity of reformer gas/air (RG) required to raise the burning velocity back to undiluted level. The burning velocity dropped from around 35 cm/s for stoichiometric methane/air mixture to about 13 cm/s if 20 % $\mathcal{V}_{SEG}$ was added to the mix. At about 20 % $\mathcal{V}_{SEG}$ fraction, 42 % $\mathcal{V}_{RG}$ was required to

bring back the burning velocity to the original undiluted level.

4.2 List of symbols



	Laminar Burning Velocity
C_P	Specific Heat at Constant Pressure
C_V	Specific Heat at Constant Volume
r_c	Compression Ratio
ν	Specific Heat Ratio (C_P/C_V)
ν_u	Specific Heat Ratio of Unburned Gases
t	Time
P	Instantaneous Pressure
P_i	Initial Pressure before Combustion
T	Temperature
T_u	Unburned Gas Temperature
EGR	Exhaust Gas Recirculation
$\mathcal{V}_{SEG}$	SEG by Volume
RG	Reformer Gas/Air
$MTEM$	Multi-Zone Thermodynamic Equilibrium Model

4.3 Introduction

The performance and safety of combustion systems depends on many parameters. Laminar burning velocity is arguably the most fundamental and important parameter describing the combustible mixture. Defined as the velocity of the flame wave with respect to quiescent unburned gases by Lewis & von Elbe [1], the laminar burning velocity scales inversely with size for continuous combustion devices like burners and inversely with combustion duration for transient combustion devices like spark ignition engines. When combustion devices have been optimized for mixtures with a particular burning velocity, it is generally disadvantageous to use mixtures with significantly different burning velocity. This situation arises with spark ignition engines where mixture dilution by Exhaust Gas Recirculation (EGR) is used to reduce peak combustion temperature and thus reduce formation of undesirable nitrogen oxides [3, 4, 5, 6]. In addition to this desirable effect, EG addition also leads to a decrease in the mixture burning velocity which contributes to longer burn duration, poor combustion phasing, greater-than-optimum heat loss and, eventually, partial burn or complete misfire of the fuel-air mixture [52, 53]. It is speculated that these undesirable side effects of EGR use could be largely avoided if the burning velocity was not affected as the mixture was diluted by EGR.

One approach to maintaining fixed burning velocity despite EG dilution is to replace part of the fuel with an alternative having a higher burning velocity. In particular, hydrogen has a high burning velocity [18, 54] and it is possible to produce substantial amounts of hydrogen by fuel reforming. Fuel reform-

ing is the process of breaking down high molar mass fuels to produce a blend of hydrogen (H_2) and carbon monoxide (CO) using a process such as partial oxidation or steam reforming [55, 56, 57]. Totally reforming a hydrocarbon fuel to H_2 and CO will typically give a burning velocity higher than the base fuel [58]. Reforming will also affect the fuel octane quality and consume some of the fuel energy. Hence, where reforming is used to maintain mixture burning velocity, it is desirable to limit the amount of reforming to the minimum required. Determining that quantity was the point of this study.

Although there is a significant amount of literature on the burning velocities of methane/air [21, 59, 19, 23, 28, 60, 61, 48] there has been little work done on methane/air/EG [28, 19]. Likewise, the effect of H_2 addition to hydrocarbon/air mixtures has been previously studied [62], however there is very little data on the effects of reformer gas addition. Since there is no way of predicting the accurate amount of reformer gas required to raise the burning velocity of the mixture back to stoichiometric level, it can be done only by trial and error. Therein lies the need to perform rigorous testing to raise the burning velocity of the methane/air/SEG mixture back to the stoichiometric methane/air level.

In this study the laminar burning velocities of methane/air/SEG/RG mixtures were measured experimentally using flame growth in a constant volume combustion chamber at initially ambient temperature and pressure. Stoichiometric mixtures were tested to reflect the chemically balanced mixtures used by spark ignition engines with "3-way" catalytic converters. Methane was

used as a base fuel and the EGR and RG compositions were simulated using pure gases to approximate the ideal combustion products and ideal reformer products of methane. The laminar burning velocities of methane/air/ SEG mixtures were measured for mixtures ranging from undiluted to the ignition limit for the spark system used. Further experimental tests were conducted to determine the degree of methane replacement by RG required to return the burning velocity of the SEG-diluted mixture to the undiluted value.

4.4 Experimental Method and Apparatus

4.4.1 Test Gas Mixtures

The methane used in the experiments was 99 % pure and dry compressed air was used. The EG was simulated by a mixture of 81.5 % N_2 (99 % pure) and 18.5 % CO_2 (99 % pure). The Reformer Gas was simulated by a mixture of 25 % CO (99.5 % pure) and 75 % H_2 (99 % pure). All percentages are composition by volume. The SEG composition was chosen based on products of stoichiometric combustion of methane and n-octane:

$$CH_4 + 2\,(O_2 + 3.773\,N_2) \longrightarrow CO_2 + 2\,H_2O + 7.546\,N_2 \qquad (4.1)$$

$$C_8H_{18} + 12.5\,(O_2 + 3.773N_2) \longrightarrow 8\,CO_2 + 9\,H_2O + 47.1625\,N_2 \qquad (4.2)$$

Since it is not practical to add water to the combustion chamber, mixture of N_2 and CO_2 was used to simulate the products of combustion. The specific heats of the mixture of N_2 and CO_2 were chosen to approximate those of

the combustion products (N_2, CO_2 and H_2O) over the range of unburned gas temperature which varies from 298 K to 388 K over the range where the burning velocity was measured. Figure 4.1. gives the specific heat of the combustion products of stoichiometric methane, n-octane and different mixtures of N_2 and CO_2 at temperatures from 298K to 388K. A mixture consisting of 81.5 % N_2 and 18.5 % CO_2 by volume, was chosen for this study as its specific heat is within 1 % of that for combustion products. It should also be noted that for true combustion, the composition of the exhaust gases remains independent to the composition of the reformer gas added to the mixture.

Although there are many methods of producing reformer gas, the steam reforming of methane based on the reaction:

$$CH_4 + H_2O_{(g)} \longrightarrow CO + 3\,H_2 \tag{4.3}$$

generates mixtures which are 25 % CO and 75 % H_2 by volume. Again, it should be noted that the percentage composition of reformer gases by volume used here is independent of the exhaust gas composition and both remained constant for all the experiments conducted. It should also be noted that when the methane/air fuel is replaced by Reformer Gas/Air, the stoichiometry is maintained by adding a stoichiometric mixture of Reformer Gas/Air (RG) mixture.

$$CO + 3\,H_2 + 2\,(O_2 + 3.773\,N_2) \longrightarrow CO_2 + 3\,H_2O + 7.546\,N_2 \qquad (4.4)$$

4.4.2 Test Cell

The main apparatus shown in Figure 3.2 consists of a constant volume cubical combustion chamber of edge length 125 mm with a central ignition point [46, 47, 48, 49, 50] (The cubical configuration was developed to allow perforated plate turbulence generation). With 25 mm thick walls, the combustion chamber can withstand peak pressures over 1400 kPa allowing initial test conditions around 202 kPa (2 atm).

A capacitive discharge/inductive coil ignition with stored energy of 110 mJ (300 V and 2.5 μf) was used for ignition. A pair of tapered spark electrodes extending from opposite sides of the chamber formed an adjustable gap at the center of the cell. A fixed 3 mm spark gap was used for all tests in this study.

A bottled gas manifold and vacuum pump attached to the system as in Figure 3.3 were used to evacuate the chamber before each run and to meter gas mixtures into the chamber by the method of partial pressures.

4.4.3 Instrumentation and Data Recording

The main pressure transducer was a flush diaphragm Precise Sensor Model 7820 using a four active arm bonded strain gage. It was calibrated using a

dead weight calibrator, and measured absolute pressures from 0 to 1725 ± 20 kPa FS (1 %). A Validyne pressure transducer with a range of 0 to 140 ± 0.7 kPa FS was used during filling and was isolated during combustion to safeguard it from high pressures. A Chromel-Alumel (Type K) thermocouple was used to measure the initial temperatures before each run.

The data acquisition is performed on a National Instruments PCI- MIO-16E-4 at a sample rate of 5 kHz. The DAQ program sends a 5 Volt pulse to the spark box to produce the spark. And then it sends another signal to the DAQ card to start recording the pressure from the pressure transducer. A delay was introduced before the signal reaches the spark box so that no data was lost due to the fact that the combustion duration is on the order of a few milli-seconds and a full pressure trace is obtained.

4.4.4 Burning Velocity Calculation Using the Multi-Zone Thermodynamic Equilibrium Model

A Multi-Zone Thermodynamic Equilibrium Model (MTEM) [49] was used to calculate the unburned mixture temperature, mass fraction burned, flame radius and burning velocity from the pressure trace, mixture composition and initial conditions. To do this, the model treats the mass of gas in the combustion chamber as 1500 concentric spherical shell elements. Combustion is modelled by the sequential burning of each element with accompanying expansion of that element, compression of all other elements and consequent pressure rise. In this model, each element is considered adiabatic from the

adjacent shells. As each of these elements burns, its flame temperature and equilibrium composition are calculated using an iterative scheme which considers only the six principal species ($CO, CO_2, O_2, N_2, H_2, H_2O$) and two principal dissociation reactions, (CO_2 dissociation and the water-gas reaction as represented by Eqns. 4 & 5).

$$CO_2 \rightleftharpoons CO + \frac{1}{2} O_2 \tag{4.5}$$

$$CO + H_2O \rightleftharpoons CO_2 + H_2 \tag{4.6}$$

It was shown by Ting [49] that these two dissociation reactions were adequate for the energy analysis of methane-air mixtures. For methane/air combustion at an equivalence ratio of 0.9, the maximum adiabatic flame temperature calculated using STANJAN [51] was 2135 K, while the temperature calculated using MTEM was 2152 K and at an equivalence ratio of 0.7, STANJAN [51] gives a value of 1839 K and MTEM gives a value of 1845 K, which accounts for a variation of less than 1 %.

The chamber shape effects are neglected because the model only focuses on the main stages of flame growth. Thus, the model can only predict the flame growth up until the time the spherical flame touches the walls of the cubical combustion chamber, after which the shape effects of the chamber begin to take control. The flame reaches the wall of the combustion chamber around the time the pressure reaches $2.2\,P_i$ (Figure 4.2), where P_i is the initial pressure. The valid data for the MTEM is then $P_i \leq P \leq 2.2\,P_i$.

From the raw pressure data, the burning velocity was calculated by using the MTEM. The burning velocity is obtained for the entire range of pressure rise. During the initial stages of combustion the fluctuation in the pressure is very high because of the electrical noise due to the spark. Since this might affect the calculation of the actual burning velocity the data from P_i to $1.05\,P_i$ was neglected. All data presented had a low signal to noise ratio.

The burning velocities corresponding to pressure from $1.05\,P_i \leq P \leq 2.2\,P_i$ is filtered by using a 7 term (± 3) moving average filter. A straight line is fitted for the filtered values using the relation given below:

$$S_u \propto (P_i/P)^{-\mu_u} \tag{4.7}$$

The points beyond (± 1) standard deviation were neglected. Once again a line is fitted for the rest of the data. The line is extrapolated to find the burning velocity of the mixture at 1 atm.

4.5 Results and Discussion

4.5.1 Confirmation of Stoichiometric Methane S_u

The burning velocity obtained for stoichiometric methane/air combustion is 34.9 cm/s. This agrees well with previous studies [22, 60, 19, 18, 20]. A comparison is given in Table 1. The agreement is better when comparison is made with studies using a constant volume closed cell [19, 18, 20]. In

particular the burning velocity is within 2.5% of that found by previous studies done using the constant volume method.

4.5.2 Decrease of S_u with SEG dilution

Typical raw pressure time series are shown in Figure 4.3 for a range of SEG/fuel mixtures. It can be noted that the mixture is stoichiometric and the initial pressure is 1 atm for all curves while dilution varies from stoichiometric to 22% $\mathcal{V}_{SEG}$. The peak pressure attained in the combustion reaction gradually decreases as the percentage $\mathcal{V}_{SEG}$ is increased (Figure 4.4). The peak pressure varies from 724 kPa at 2% $\mathcal{V}_{SEG}$ to 555 kPa at 22% $\mathcal{V}_{SEG}$. In Figure 4.4 the ratio of $\frac{P_{max}}{P_o}$ is plotted against percentage $\mathcal{V}_{SEG}$. A linear fit of the local maxima in Figure 4.4 yields a value of 10.75 for $\frac{\frac{dP_{max}}{dP_o}}{d\mathcal{V}_{SEG}}$.

In Figure 4.5 the time for the reaction to attain peak pressure is plotted against the fraction of $\mathcal{V}_{SEG}$. The reaction time increases as the percentage of $\mathcal{V}_{SEG}$ goes up, indicating that the burning velocity decreases as more SEG is added to the mixture. It is notable that the combustion time increases at a greater than linear rate as SEG is added and the time to peak pressure more than doubles (from 90 ms to 235 ms) as sufficient SEG is added to reach the ignition limit. It was found that the mixture could burn at $\mathcal{V}_{SEG}$ levels as high as 22%. But it stopped burning at 23% $\mathcal{V}_{SEG}$.

As expected, the burning velocity decreases gradually with the addition of $\mathcal{V}_{SEG}$ Figure 4.6. The burning velocity with 2% $\mathcal{V}_{SEG}$ is around 30 cm/s and for 22% $\mathcal{V}_{SEG}$ it is around 11 cm/s. A linear fit yields a burning velocity

Table 4.1: Comparison of stoichiometric methane/air burning velocities with previous studies.

No.	Previous Study	Method	S_u cm/s
1	Bosschaart, K. J. et al [22]	Heat flux method	36
2	Gu, X. J. et al [60]	Constant Pressure	35.8
3	Clarke, A. et al [19]	Closed Cell	35.4
4	Iijima, T. et al [18]	Closed Cell	35
5	Hassan, M. I. et al [20]	Closed Cell	35
5	This study	Closed Cell	34.9

variation of -1.9 cm/s for each percentage $\mathcal{V}_{SEG}$ increase. In non-dimensional terms, this would be a 3 % reduction of undiluted burning velocity for each percent of $\mathcal{V}_{SEG}$ added.

The fall in burning velocity with the addition of SEG is as expected. This is attributed to the decrease in the flame temperature as more SEG is added. With the addition of SEG to the mixture the specific heat capacity of the mixture increases when compared to the stoichiometric methane/air mixture resulting in a lower burning velocity.

4.5.3 RG addition to required maintain S_u

When compared with the previous studies, at 5 % $\mathcal{V}_{SEG}$ the burning velocity was 28 cm/s in this study while it was 25 cm/s for Elia et al [28] and 28 cm/s for Clark et al [19], at 15 % $\mathcal{V}_{SEG}$ it was found to be 16 cm/s in this study and 11cm/s for Elia et al [28] and 17 cm/s for Clark et al [19].

As the reformer gas is added to the mixture the flame temperature increases which results in higher burning velocities. It is also noted that the flame temperature is still lower than pure methane/air flame temperatures. Again with the addition of the reformer gas, the specific heat decreases which in turn leads to higher flame temperatures and higher burning velocities. The exhaust gas recirculation and reformer gas addition can be incorporated to stationary engines running on methane/air and can be extended to automobiles once on-board reforming can be optimized. This will result in the

possibility of using higher compression ratios and less NO_X emissions.

The percentage of reformer gas required to raise the burning velocity to undiluted levels at different levels of dilution with $\mathcal{V}_{SEG}$ is shown in Figure 4.7. It was found that with 4 % $\mathcal{V}_{SEG}$ mixture, 14 % $\mathcal{V}_{RG}$ was required to raise the burning velocity back to the undiluted level and for 22 % $\mathcal{V}_{SEG}$, it took about 42 % $\mathcal{V}_{RG}$ to restore the burning velocity. The burning velocity was raised to 34.24 cm/s with a standard deviation of 1.3 at 95 % confidence levels 34.24 $\pm$ 1.3 cm/s (2σ) as shown in detail in Figure 4.8. When the ratio of percentage $\mathcal{V}_{RG}$ to that of the percentage $\mathcal{V}_{SEG}$ was considered it was about 3.5 for 4 % $\mathcal{V}_{SEG}$, gradually decreasing to 2.5 for 8 % $\mathcal{V}_{SEG}$ and stabilizing at 2.1 for 12 % to 20 % $\mathcal{V}_{SEG}$ levels. A linear fit gives an equation

$$\mathcal{V}_{RG} = 1.75 * \mathcal{V}_{SEG} + 6.3 \tag{4.8}$$

This equation applies to $\mathcal{V}_{SEG}$ percentages from 2 to 20.

4.6 Conclusion

Laminar burning velocities of various mixtures of methane, air, SEG and RG have been measured in a cubical combustion chamber with an initial temperature of 298 K and an initial pressure of 1 atm.

The burning velocity of the stoichiometric methane/air mixture was found to be 34.9 cm/s. The burning velocity gradually decreased as SEG was added

to the mixture. When SEG replaced 4 % of the methane/air the burning velocity dropped to 28 cm/s. This trend continued, as 16 % $\mathcal{V}_{SEG}$ resulted in a burning velocity of 16 cm/s. The change in the burning velocity decreases slightly with higher $\mathcal{V}_{SEG}$ fractions, 20 % $\mathcal{V}_{SEG}$ gave a burning velocity of 13 cm/s. The mixture failed to ignite at $\mathcal{V}_{SEG}$ fractions higher than 20 %.

The percentage by volume of RG required to raise the burning velocity back to undiluted levels varies with the percentage of $\mathcal{V}_{SEG}$ used. At 4 % $\mathcal{V}_{SEG}$ level, 14 % $\mathcal{V}_{RG}$ was required. This trend continues linearly to an $\mathcal{V}_{SEG}$ fraction of 20 % requiring 42 % $\mathcal{V}_{RG}$ to restore the original undiluted burning velocity.

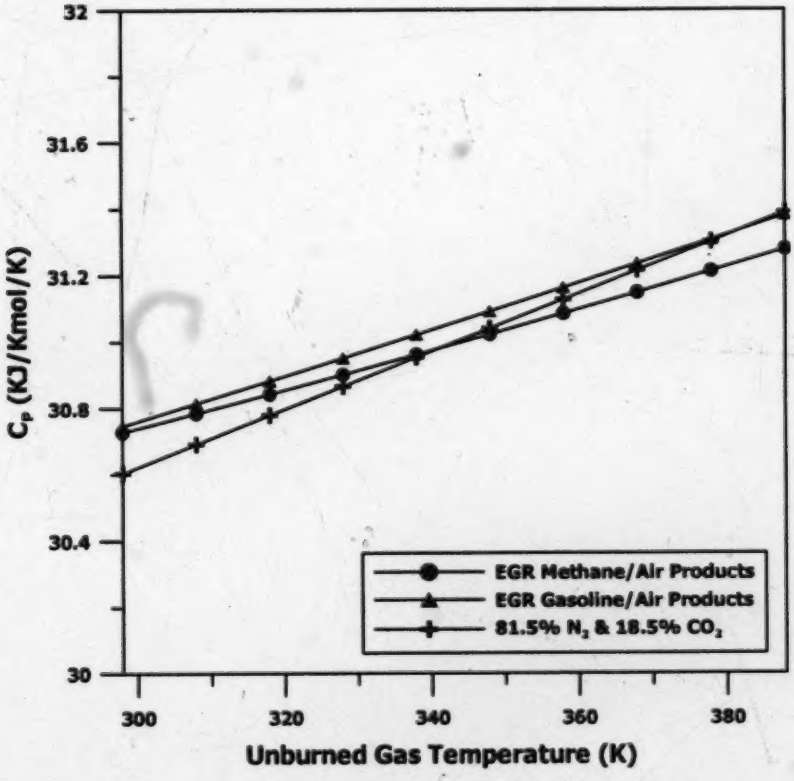


Figure 4.1: The variation of specific heat for combustion products and simulated EG mixture over a temperature range typical of the unburned gas in a combustion test chamber

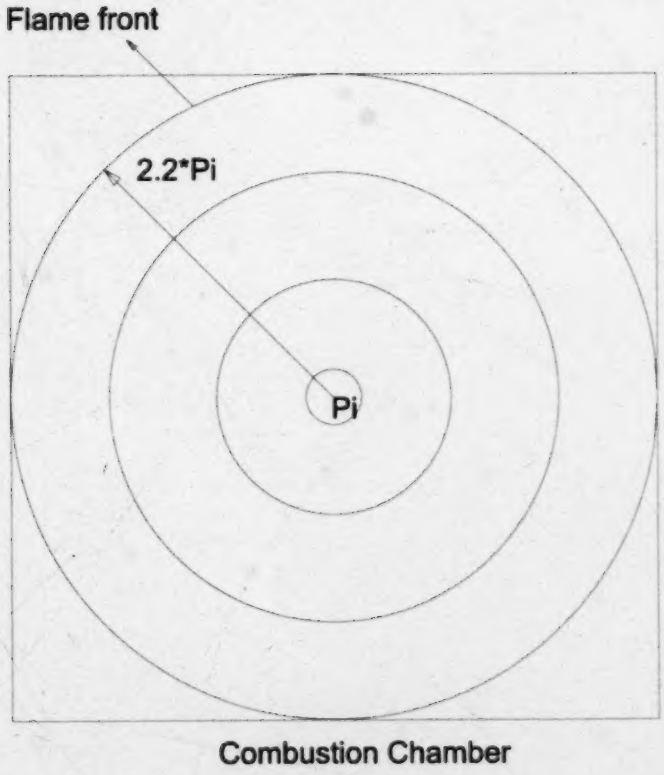


Figure 4.2: A Spherical flame growing in a Cubical Cell contacts the wall when pressure is $2.2\,P_i$

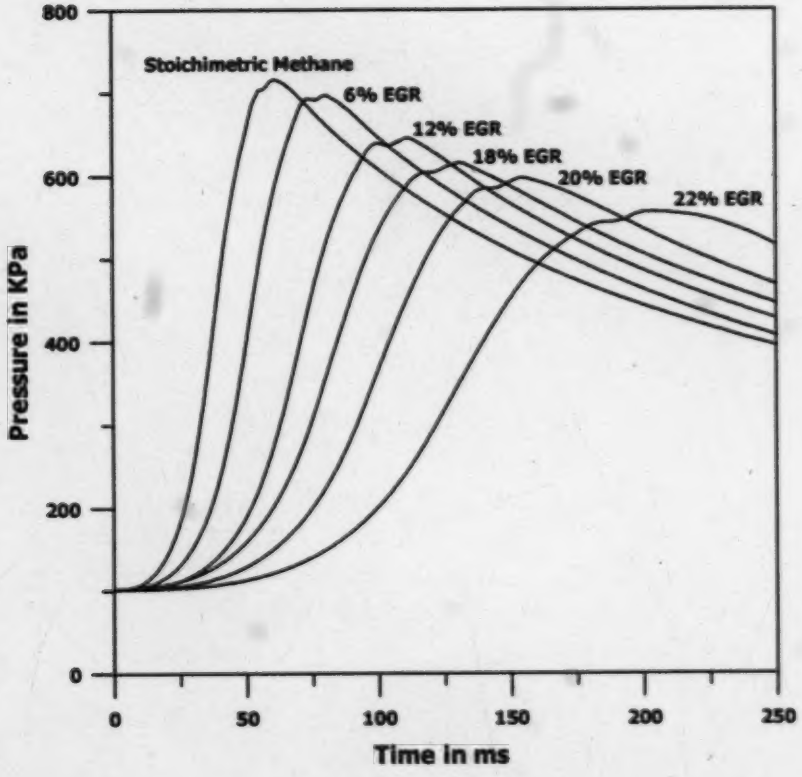


Figure 4.3: Raw pressure traces for stoichiometric methane-air mixtures with varying dilution by simulated exhaust gases ($P_i = 1$ atm, $T_i = 298$ K)

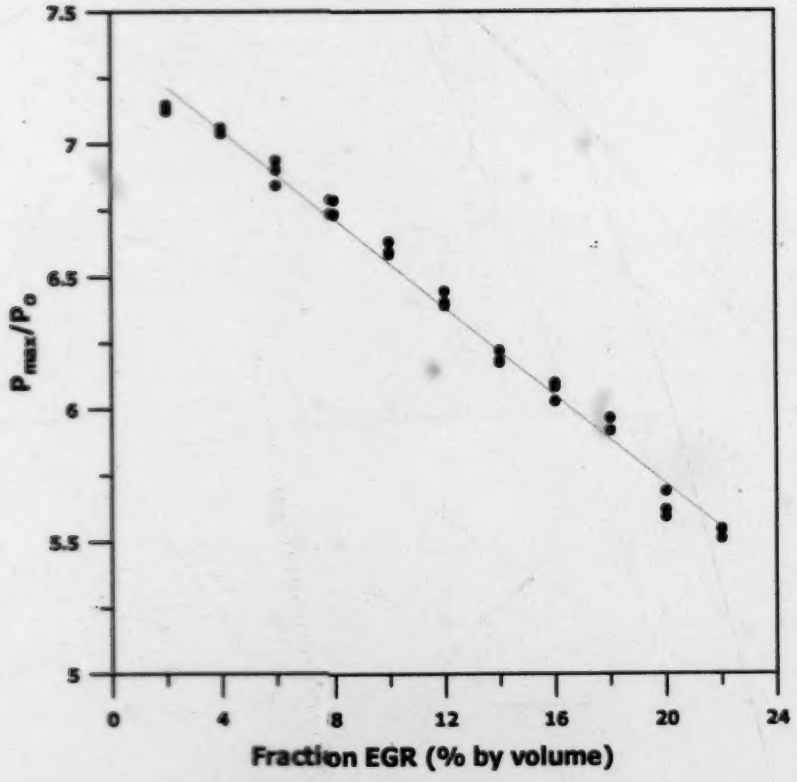


Figure 4.4: Effect of increasing exhaust dilution on Peak Combustion Pressure ($P_i = 1$ atm, $T_i = 298$ K)

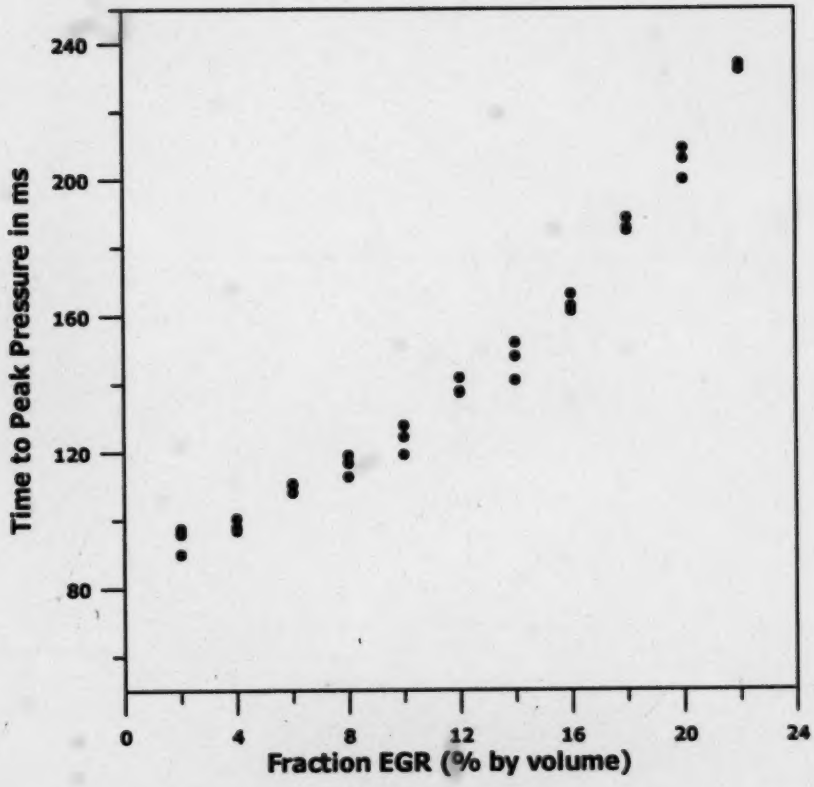


Figure 4.5: Effect of increasing exhaust gas fraction on time to attain peak combustion pressure (Stoichiometric methane-air mixtures, $P_i = 1$ atm, $T_i = 298$ K)

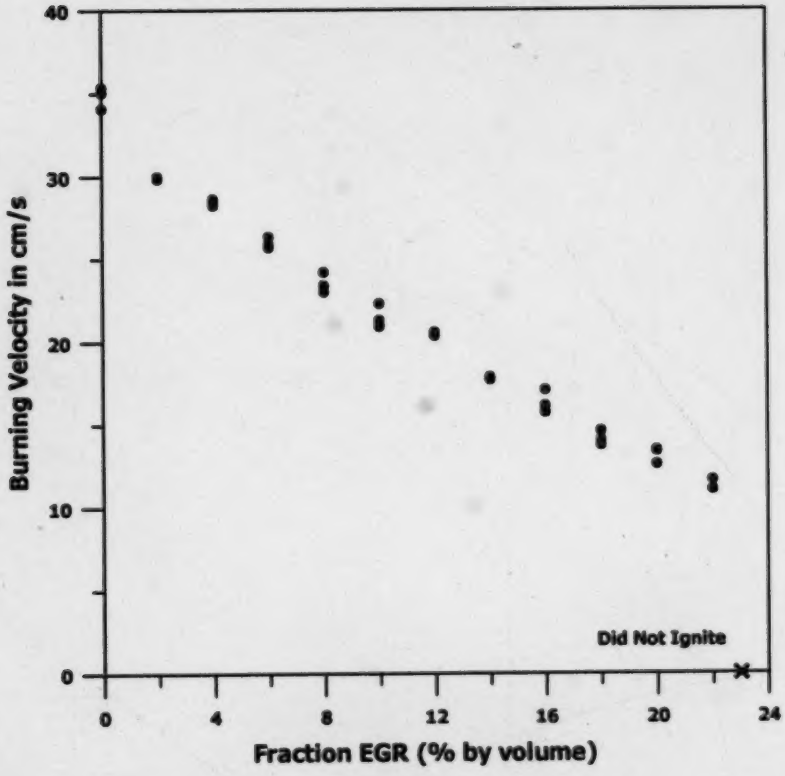


Figure 4.6: The reduction of burning velocity with increasing exhaust gas fraction for stoichiometric methane-air mixtures ($P_i = 1$ atm, $T_i = 298$ K)

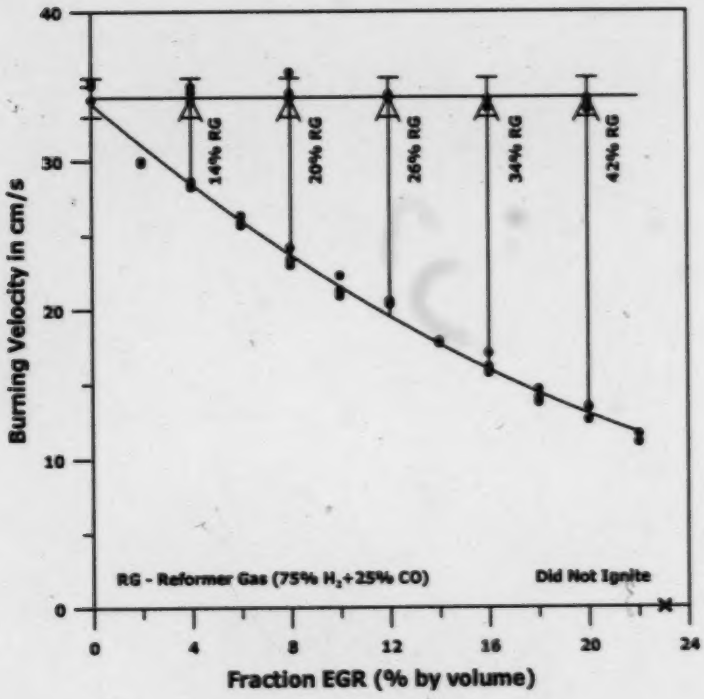


Figure 4.7: Amount of reformer gas required to restore burning velocity to undiluted methane-air levels; Error bars show 95 % confidence in burning velocity ($P_i = 1$ atm, $T_i = 298$ K)

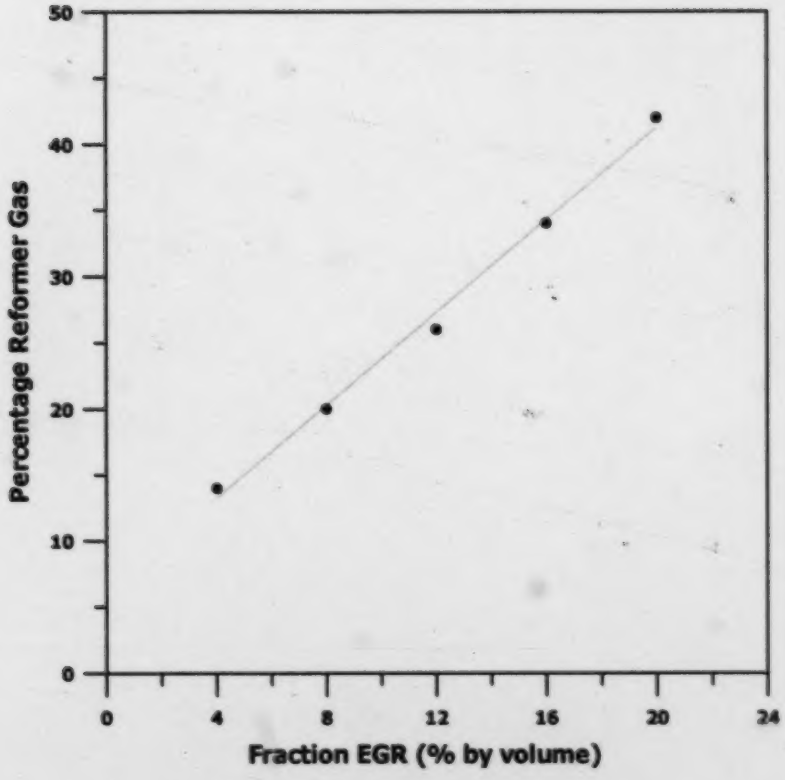


Figure 4.8: Relationship between reformer gas fraction required to restore the burning velocity to undiluted methane-air and exhaust gas dilution level

Chapter 5

Burning velocities of laminar premixed Carbon monoxide-Hydrogen-Air mixtures - Journal of Automobile Engineering, To be submitted

5.1 Abstract

This study presents the burning velocities of hydrogen (H_2)-carbon monoxide (CO)-air mixtures over a range of H_2 and CO volume fractions. There is very little literature available on a varied range of H_2/CO-air mixture. The equivalence ratios were varied from 0.6 to 1.6 in the present study. The experiments are conducted in a constant volume cubical combustion chamber. The laminar burning velocity (S_u), unburned mixture temperature, mass fraction burned and the flame radius are calculated by the Lewis and von Elbe method and Multi-zone Thermodynamic Equilibrium Model (MTEM) from the pressure trace. S_u is obtained for different fuel compositions and equivalence ratios at 1 atm and 296 K. S_u of stoichiometric H_2 from the Lewis

and von Elbe model was found to be 207 cm/s and that from the MTEM was found to be 192 cm/s, The S_u of stoichiometric, equi-molar CO-H_2 mixture was found to be 107 cm/s using Lewis and vol Elbe and 100 cm/s using MTEM. This study also covers a whole range of H_2 fraction (0-100 %) in the fuel.

5.2 List of symbols

S_u	Laminar Burning Velocity
C_P	Specific Heat at Constant Pressure
C_V	Specific Heat at Constant Volume
r_c	Compression Ratio
ν	Specific Heat ratio (C_P/C_V)
ν_u	Specific Heat ratio of Unburned Gases
t	Time
P	Pressure at any instant, t
P_i	Initial Pressure before Combustion
P_e	Final Pressure
T	Temperature
T_u	Unburned Gas Temperature
EGR	Exhaust Gas Recirculation
$MTEM$	Multi-Zone Thermodynamic Equilibrium Model
LHV	Lower Heating Value
$\mathcal{V}_H$	Percentage Hydrogen by Volume
$\mathcal{V}_{CO}$	Percentage Carbon monoxide by Volume
$\mathcal{V}_A$	Percentage Air by Volume

5.3 Introduction

The laminar burning velocity, defined as the velocity of the flame wave with respect to quiescent unburned gases by Lewis & von Elbe [1], is the most important parameter of a combustible mixture. The knowledge of burning velocity of an air-fuel mixture is of paramount importance if the mixture is to be used in any kind of combustion system, since almost all the combustion properties of gas mixtures are dependent on the burning velocity. Any given combustion device is designed to work the most efficient with a specific fuel in mind with a fixed burning velocity. The efficiency tends to decrease as the burning velocity is decreased. In the case of EGR addition to fuels the burning velocity drops down considerably. It has been shown that the laminar burning velocity of methane-air mixture drops by 1.9 cm/s (In non-dimensional terms, this would be a 3 % reduction of undiluted burning velocity for each percent of EGR added) for each volume % of EGR increase [63]. The decrease in the mixture burning velocity can contribute to longer burn duration, poor combustion phasing, heat loss, partial burn or complete misfire of the fuel-air mixture [52, 53]. This can be prevented by replacing the actual fuel with another having a higher burning velocity than the primary fuel, and hydrogen is the best viable option as it can sustain vigorous burning under lean conditions.

The production of H_2 for use in such cases is done by steam reforming of methane or other light hydrocarbons (ethane or propane) in the presence of a catalyst or by partial oxidation of hydrocarbons (such as natural gas, naphtha, petroleum coke or coal) or by the combination of both (autothermal

reforming). Approximately 96 % of the H_2 produced in the world is by some form of steam reforming of carbonaceous fuel. In all the above mentioned cases, CO is obtained as a byproduct. The CO can be removed by water-gas shift reactions and H_2 recovery. However, these processing steps add a significant cost to H_2 production. In the case of S.I. engines, the CO-H_2 mixture (Reformer Gas) can be used directly, without bothering to remove the CO, as it simply increases the available energy in the fuel. This makes knowledge of the burning velocities of CO-H_2-air mixtures important, and generating such knowledge is the purpose of this study.

There is very little data on the burning velocities of a varied range of CO-H_2-air mixtures. Scholte et al. [39] studied the burning velocities of binary CO-H_2 mixtures using the burner method. However, all their mixtures were rich, using up to 50 % fuel by volume in their experiments. McLean et al. [40] studied 95 % CO + 5 % H_2 and equimolar mixture of CO-H_2 at different equivalence ratios, although their primary objective was to determine the rate of CO + OH reaction. Vagelopoulos et al. [40] studied the burning velocity of very lean mixtures (80 % air) of CO-H_2 at different H_2 mole fractions. Linteris [41] studied the burning velocity of premixed CO-Ar-O_2-H_2 flames inhibited by CF_3H using the burner method. Brown et al. [42] measured the Markstein lengths of three fuel mixtures: 95 %-5 % CO-H_2, 50 %-50 % CO-H_2 and 100 % H_2. Hassan et al. [43] studied the effects of positive stretch on the laminar burning velocities in CO-H_2-air mixtures. They went from 3-50 % H_2 in the fuel and equivalence ratios from 0.6-5. Rightley et al [44] investigated the laminar burning velocities of CO-O_2 along with an inert and

trace amounts of H_2 containing species. El-Sherif [64] studied the control of emissions using H_2-CO additive to methane-air flames. Linteris et al. [65] studied the burning velocity of premixed CO-NO flames from equivalence ratio 0.6 to 3, with trace amounts of H_2. Rumminger et al. [45] investigated the burning velocity of CO-H_2-O_2-N_2 with and without Iron Pentacarbonyl over a range of O_2 and H_2 fractions using the burner method. In short a varied range of CO-H_2-air mixtures have not been studied by methodically varying the equivalence ratios and also the fraction of H_2 in the CO-H_2-air mixtures. This is the exact objective of this study.

5.4 Experimental Method and Apparatus

The main apparatus (Figure 3.2) consists of a constant volume cubical combustion chamber of edge length 125 mm with a central ignition point [63, 46, 47, 48, 49, 50]. (The cubical configuration was developed to allow perforated plate turbulence generation). It has 25 mm thick aluminium walls, and can withstand peak pressures over 1400 kPa. A capacitive discharge/inductive coil ignition with stored energy of 110 mJ (300 V and 2.5 μF) was used for ignition. A pair of electrodes which can be moved relative to one another provide an adjustable spark gap at the center of the cell. The spark gap was maintained at 3 mm for all the tests in this study.

A vacuum pump attached to the system (Figure 3.3) was used to evacuate the chamber before each run. A bottled gas manifold was attached to meter gas mixtures into the chamber by the method of partial pressures. The H_2

and CO used in the experiments were over 99 % pure and dry compressed air was used.

The pressure transducer used to measure the pressure rise was a flush diaphragm Precise Sensor Model 7820 using a four active arm bonded strain gage and it measured absolute pressures from 0 to 1725 ± 20 kPa (1 %). It was calibrated using a dead weight calibrator. To measure the partial pressures of gases when they were added to the cell, a Validyne pressure transducer with a range of 0 to 140 ± 0.7 kPa was used during filling. It was isolated during combustion to safeguard it from high pressures. Care was taken so that the pressure in the gas manifold was always higher than the pressure in the chamber so that there was no possibility of back flow occurring. A similar Validyne pressure transducer was attached to the gas manifold to facilitate this. A Chromel-Alumel thermocouple was used for measuring the initial gas temperatures before each run and during filling to ensure partial pressures were not affected by gas cooling as it expanded into the combustion cell. Pressure traces were recorded using a personal computer equipped with a data acquisition card (National Instruments PCI- MIO-16E-4) at a data rate of 10 KHz. For a more detailed explanation of the apparatus refer to Ponnusamy et al. [63].

5.5 Burning Velocity Calculation

The burning velocity was calculated from the pressure traces using two methods:

5.5.1 Lewis and von Elbe

The burning velocity, unburned mixture temperature, mass fraction burned and the flame radius are calculated by the Lewis and von Elbe method [1] from the time-pressure trace. The procedure is briefly explained below. Say a fraction n of gas before ignition occupies a sphere of volume V_i and radius r_i and after combustion gives rise to a pressure P and if a is the hydraulic radius of the vessel if it were a sphere, T_i the temperature before ignition, T_u is the unburned gas temperature, P_e is the equilibrium pressure calculated from STANJAN [1] [51], then

$$r_i = a\left(\frac{P-P_i}{P_e-P_i}\right)^{\frac{1}{3}} \tag{5.1}$$

If the volume of the fraction n after burning is V_b and its radius r_b, then

$$r_b = a\left(1 - \frac{P_i}{P}\frac{T_u}{T_i}\frac{P_e-P}{P_e-P_i}\right)^{\frac{1}{3}} \tag{5.2}$$

Now using the two equations given above the burning velocities and the flame speed can be determined. The flame speed can be obtained by finding out the slope of dr_b/dt and the burning velocity is obtained by the equation,

$$S_u = \frac{dr_b}{dt}\left(\frac{r_i}{r_b}\right)^2\left(\frac{P_i}{P}\right)^{\frac{1}{\kappa_u}} \tag{5.3}$$

[1] STANJAN is an interactive program for chemical equilibrium analysis by the method of element potentials. It handles a gas phase and multiple condensed phases. The JANNAF thermochemical tables are used as the primary data base. Each phase is modelled either as a mixture of ideal gases or an ideal solution.

5.5.2 Multi-Zone Thermodynamic Equilibrium Model

The burning velocity, unburned mixture temperature, mass fraction burned and the flame radius are calculated by the Multi-Zone Thermodynamic Equilibrium Model (MTEM) [49] from the pressure trace, the mixture composition and the initial conditions. The MTEM divides the mass of gas inside the cubical chamber into 1500 concentric spherical shell elements. The combustion is modelled by sequential burning of elements causing expansion of the element which leads to the compression of the rest of the elements and therefore a pressure rise. Each of the spherical elements is considered to be sealed from the adjacent elements. As the sequential burning occurs, the flame temperature and equilibrium composition are calculated using an iterative scheme consisting of six principal species (CO, CO_2, O_2, N_2, H_2, H_2O), and two reactions namely CO_2 dissociation and the water-gas reactions.

$$CO_2 \rightleftharpoons CO + \frac{1}{2} O_2 \tag{5.4}$$

$$CO + H_2O \rightleftharpoons CO_2 + H_2 \tag{5.5}$$

These two dissociation reactions were found to be adequate for the energy analysis of methane-air mixtures. For methane/air combustion at an equivalence ratio of 0.9, the maximum adiabatic flame temperature calculated using STANJAN [51] was 2135 K, while the temperature calculated using MTEM was 2152 K and at an equivalence ratio of 0.7, STANJAN [51] gives a value of 1839 K and MTEM gives a value of 1845 K, which accounts for a variation of less than 1 %. Since the study focuses only on the main stage of flame

propagation, before the flame strikes the wall, the chamber shape effects were neglected. After the flame touches the walls of the chamber, the flame is no longer spherical. The time for the flame to reach the walls of the combustion chamber is approximately the same time for the pressure to reach $2.2\,P_i$ (Figure 4.2).

The burning velocity was calculated by using the MTEM to analyze the pressure data. The burning velocity calculation is applied for the entire range of pressure rise. During the initial stages of combustion the fluctuation in the pressure is very high because of the noise due to the spark. Since this might affect the calculation of the actual burning velocity, the data from P_i to $1.05\,P_i$ was neglected. Only runs with low signal to noise ratio were included in the results presented in this study. The burning velocities corresponding to pressure from $(1.05 - 2.2)\,P_i$ are filtered by using a 7 term (± 3) moving average filter.

A straight line is fitted for the filtered values using the relation given below:

$$S_u \propto \left(\frac{P_i}{P}\right)^{\frac{1}{n}} \tag{5.6}$$

The points beyond (± 1) Standard Deviation were neglected. Once again a line was fitted for the rest of the values and was extrapolated to find the burning velocity of the mixture at 1 atm.

5.6 Results and Discussion

The pressure traces obtained when stoichiometric CO-air, stoichiometric H_2-air and an equal mix of stoichiometric CO-H_2-air are shown in Figure 5.1 As expected the stoichiometric reaction of H_2-air was the fastest reaching the peak pressure of 718 kPa in 22.7 ms, while it took 49.4 ms for an equal CO-H_2-air mix to reach a peak pressure of 697 kPa and 222 ms for stoichiometric CO-air to reach a peak pressure of 651 kPa. So when compared with the time to peak pressure for stoichiometric H_2, it took more than twice the time for stoichiometric CO-H_2 and more than 10 times the time for stoichiometric CO to reach the peak pressure.

5.6.1 Comparison of the Models

The Lewis and von Elbe model assumes negligible pressure rise and density change so it becomes less accurate for significant pressure rise, therefore the Multi Zone Thermodynamic Equilibrium Model is more accurate than the Lewis and von Elbe model. The average difference in the burning velocities obtained from the two models is around 7%. The variation in the burning velocity noted between the two models could be due to the difference in the assumptions the models make. The burned mass fraction is assumed to be a function of pressure in the case of Lewis and von Elbe model. The MTEM uses a geometric method while calculating the flame radius. The thermodynamic properties varying with pressure and temperature are taken into consideration in the case of the MTEM. The MTEM accounts for the dissociation reaction in terms of CO_2 dissociation and water gas reaction.

It also considers equilibrium calculation and energy balance on the burning element. So the MTEM is considered more accurate compared to the Lewis and von Elbe model.

5.6.2 Burning Velocities of Hydrogen-Air Mixtures

The laminar burning velocities of various hydrogen-air mixtures are given in Figure 5.2, with the laminar burning velocities obtained by both Lewis and von Elbe method and MTEM plotted against the equivalence ratio. The results were also compared with the works of Qin et al. (Particle Tracking Velocimetry) [66], Aung et al. (Spherical Bomb) [67], Koroll et al. (Double Kernal Technique) [68] and Dowdy et al. (High Speed Schlieren Imaging) [54]. The curve takes a concave upwards trend, with the burning velocity increasing from around 120 cm/s at an equivalence ratio of 0.6 to 207 cm/s at an equivalence ratio of 1 and 296 cm/s at an equivalence ratio of 1.6.

When the flame temperatures obtained using STANJAN [51] with initial conditions of 298 K and 1 atm are plotted against the equivalence ratio, again a concave upwards trend is obtained. This might have a little effect on the final burning velocity, but the effect of heating value of the fuel in the fuel/air mixture and the heating value of the fuel is more pronounced and seems to take over in the resulting burning velocities. As the burning velocity pretty much linearly increases with increasing heating value. The flame temperature and the lower heating value of H_2 in the fuel/air mixture is plotted in Figure 5.3.

5.6.3 Burning Velocities of stoichiometric Carbon monoxide- Hydrogen mixtures

The laminar burning velocities of stoichiometric CO-H_2, with varying levels of H_2 in the fuel are given in Figure 5.4. It should be noted that the equivalence ratio is maintained at 1 through out in this set of experiments. When the burning velocity is plotted against the percentage of H_2 in the fuel, an almost linear trend is obtained, with the burning velocity of Stoichiometric CO at 29 cm/s to 207 cm/s for stoichiometric H_2. A linear fit yields the following equation with an R^2 value of 0.99185 for the Lewis and von Elbe method:

$$S_u = (1.77\,\mathcal{V}_H \text{ in fuel} + 25.88)\,\text{cm/s} \tag{5.7}$$

and another linear fit for the MTEM values yields

$$S_u = (1.65\,\mathcal{V}_H \text{ in fuel} + 23.61)\,\text{cm/s} \tag{5.8}$$

with an R^2 value of 0.993835.

The results were compared to Hassan et al. (1997) [43], McLean et al. (1994) [40] and Gunther et al. (1971) [69] and the comparison is also given in Figure 5.4. The results seemed to agree fairly well with the previous studies. When the flame temperature obtained from STANJAN [51] was plotted against the percentage of H_2 in the fuel a concave upwards trend is obtained.

This is shown in Figure 5.5. The LHV of Fuel is also plotted against the percentage H_2 in the fuel and the trend in that case is linear.

In the Figure 5.6, the time taken to reach 2.2 P_i and the time taken to reach peak pressure in the combustion chamber are plotted against the percentage of hydrogen in the fuel. For stoichiometric CO, i.e., with no hydrogen the time to reach 2.2 P_i was 32.5 ms. While for stoichiometric hydrogen the time to 2.2 P_i was only about 4.2 ms.

5.6.4 Burning Velocities of Carbon monoxide-Hydrogen mixtures

Experiments were conducted for different air-fuel mixtures, with the volume percentages varying from 80 % to 60 %. The laminar burning velocity values for all of these different air-fuel mixtures with varying H_2 fractions are plotted in Figures 5.6.4 and 5.6.3. The burning velocities are plotted against $\frac{(LHV of H_2)}{(LHV of Fuel)}$. At 70 % Air with increasing $\frac{(LHV of H_2)}{(LHV of Fuel)}$ the burning velocity also increases linearly, while for less than 70 % air (60 % and 65 %) the increase in the burning velocity takes a concave upwards trend and for more than 70 % air (75 % and 80 %) the increase in the burning velocity takes a concave downwards trend. It should also be noted that at 70 % air the air-fuel ratio is always maintained at stoichiometric value. But the equivalence ratio changes at all other volume percentages of air. The burning velocities are plotted against volume percentage of H_2 at different air-fuel ratios in Figure 5.9. The effect of H_2 and air on the burning velocities of the CO-H_2 is shown in Figure 5.10. Almost all of the different H_2 curves show a linear trend.

5.7 Conclusion

The purpose of this study was to measure the laminar burning velocities of a varied range of CO-H_2-air mixtures. The lLaminar burning velocities of mixtures of H_2-air and CO-H_2-air have been measured in a cubical combustion chamber with initial temperature at 298 K and initial pressure at 1 atm. The volume fraction of air was varied from 60-80 % in increments of 5, the equivalence ratio varied from 0.6 to 1.6 and the fraction of H_2 in fuel from 0-100 %. The resulting data set is expected to be useful for practical and modelling purposes.

Burning velocity of stoichiometric H_2 from the Lewis and von Elbe model was found to be 207 cm/s and that from the MTEM was found to be 192 cm/s. The burning velocity gradually decreases as CO is added to the mixture. For pure CO, the burning velocity drops to around 29 cm/s (Lewis and von Elbe) and 27 cm/s (MTEM).

The burning velocity at an equivalence ratio of 1 for different $\mathcal{V}_H$ was also measured. The burning velocity increases from about 29 cm/s for 0 % $\mathcal{V}_H$ (i.e., pure CO) to about 107 cm/s for 15 % $\mathcal{V}_H$ (i.e., equi-molar CO-H_2 and about 207 cm/s for 30 % $\mathcal{V}_H$ (pure H_2). The burning velocity values obtained from the MTEM model was found to be around 7% lower than that obtained

from the Lewis and von Elbe model.

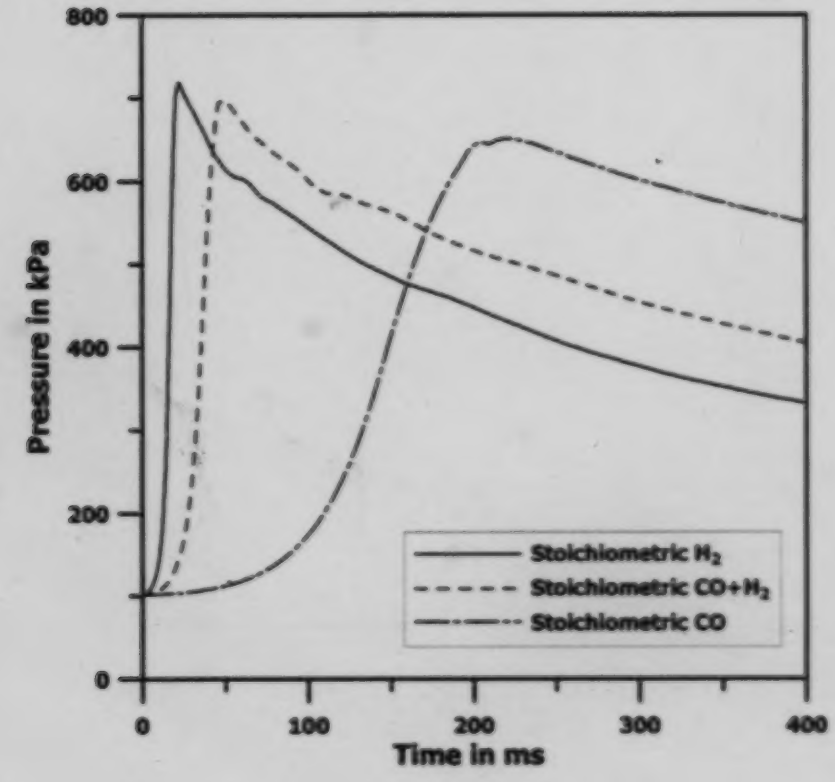


Figure 5.1: Pressure traces for stoichiometric mixtures of hydrogen, equi-molar carbon monoxide-hydrogen, stoichiometric carbon monoxide with air ($P_i = 1$ atm, $T_i = 298$ K)

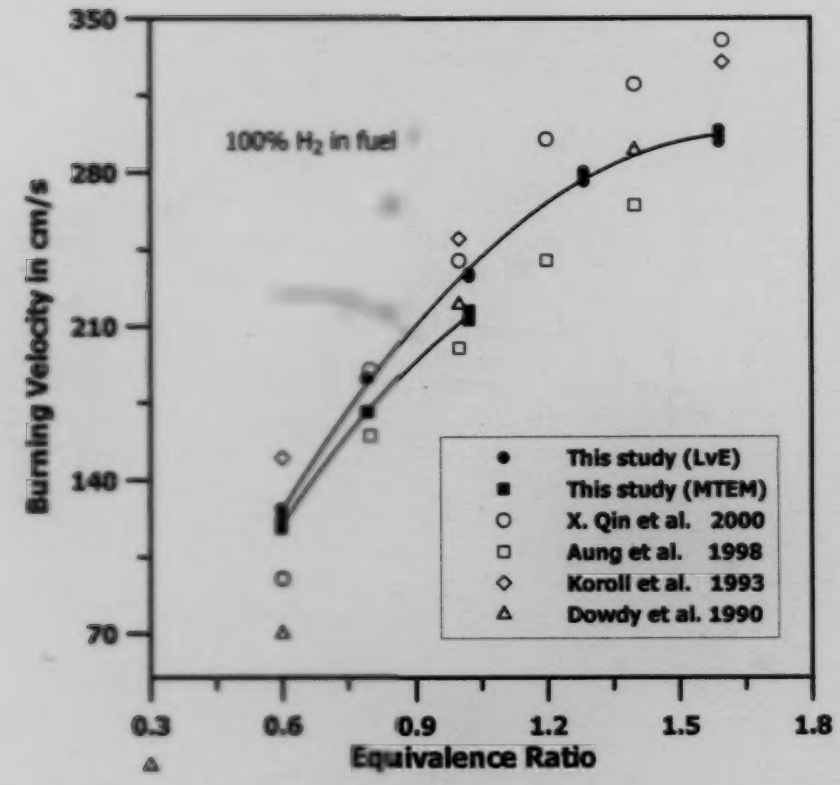


Figure 5.2: Burning velocities of Hydrogen at different equivalence ratios

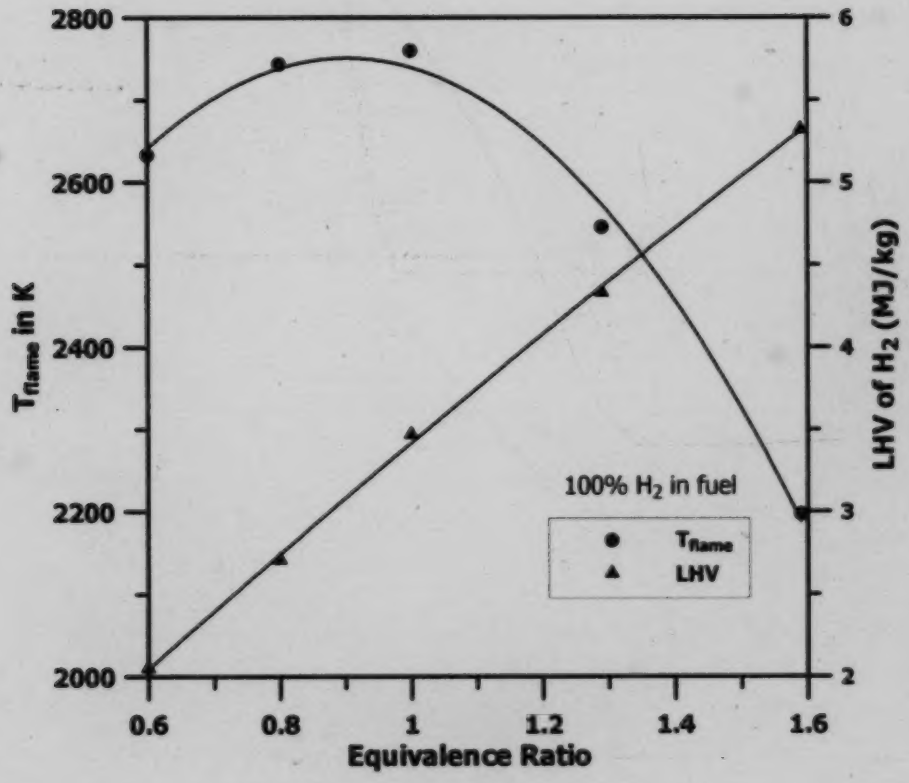


Figure 5.3: Variation of adiabatic equilibrium flame temperature and LHV of Hydrogen in air-fuel mixture with equivalence ratios for Hydrogen ($P_i = 1$ atm, $T_i = 298$ K)

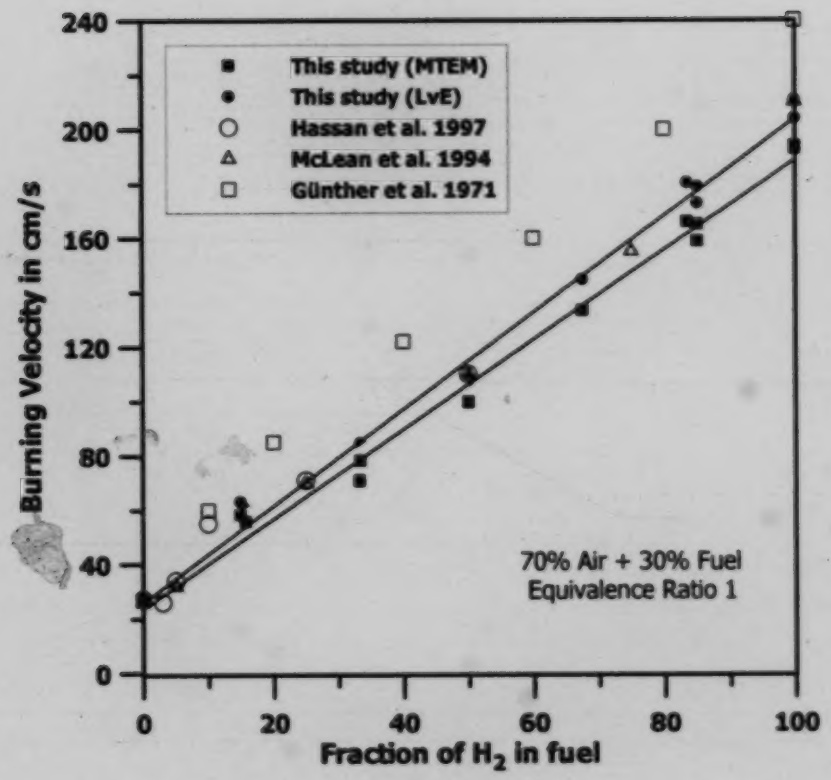


Figure 5.4: Burning velocities of Carbon monoxide-Hydrogen-Air mixtures with varying Hydrogen fraction in fuel at an equivalence ratio of 1

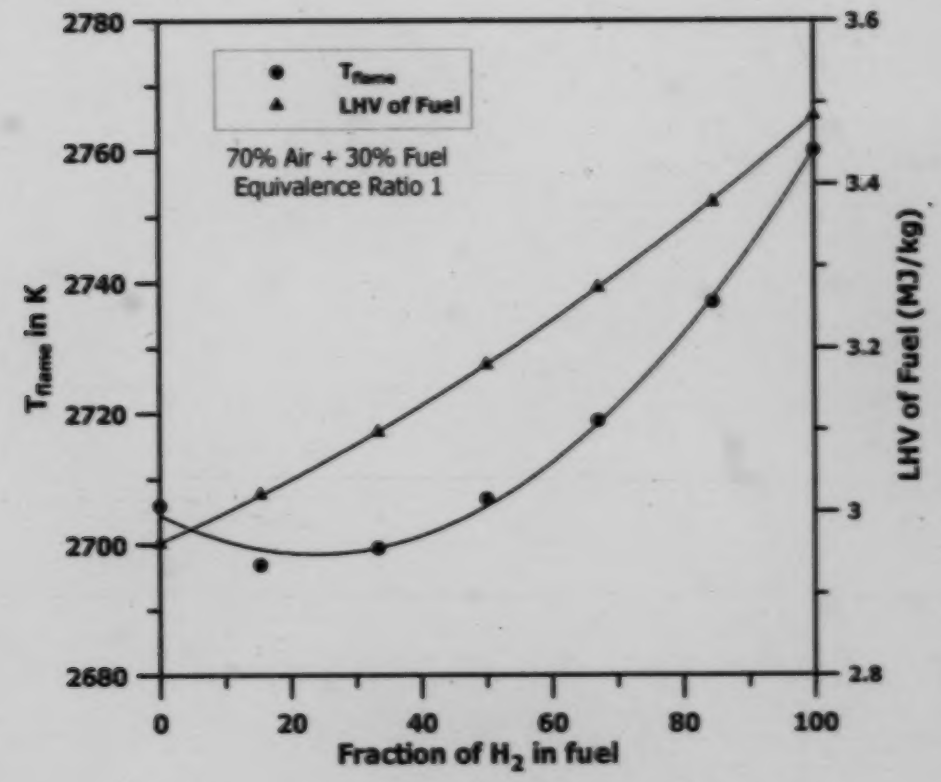


Figure 5.5: Variation of adiabatic equilibrium flame temperature and LHV of fuel with hydrogen fraction in the carbon monoxide-hydrogen mixture at an equivalence ratio of 1 ($P_i = 1$ atm, $T_i = 298$ K)

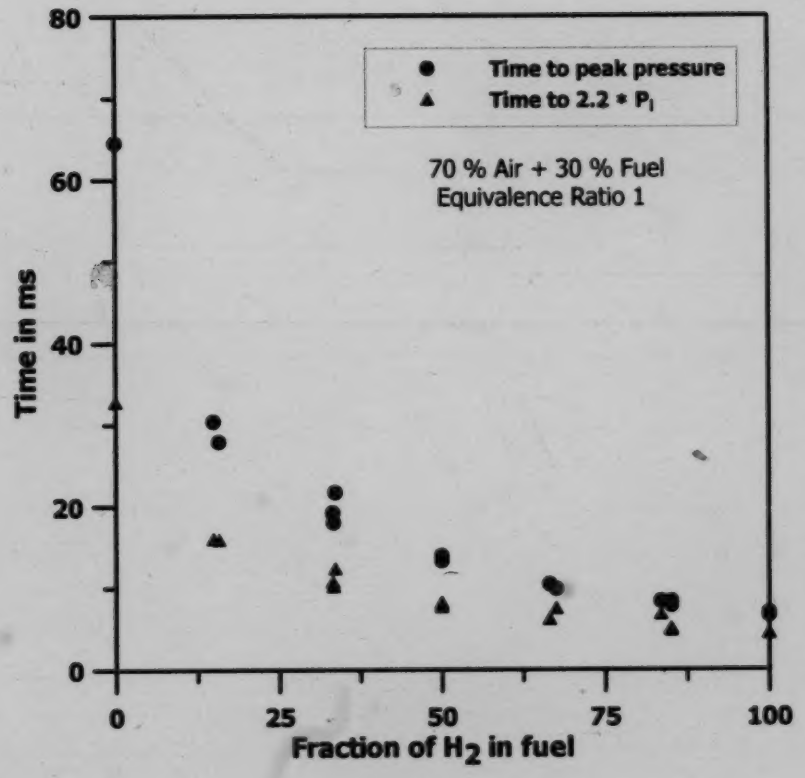


Figure 5.6: Effect of increasing Hydrogen fraction on time to attain peak combustion pressure and time to attain 2.2 P_i

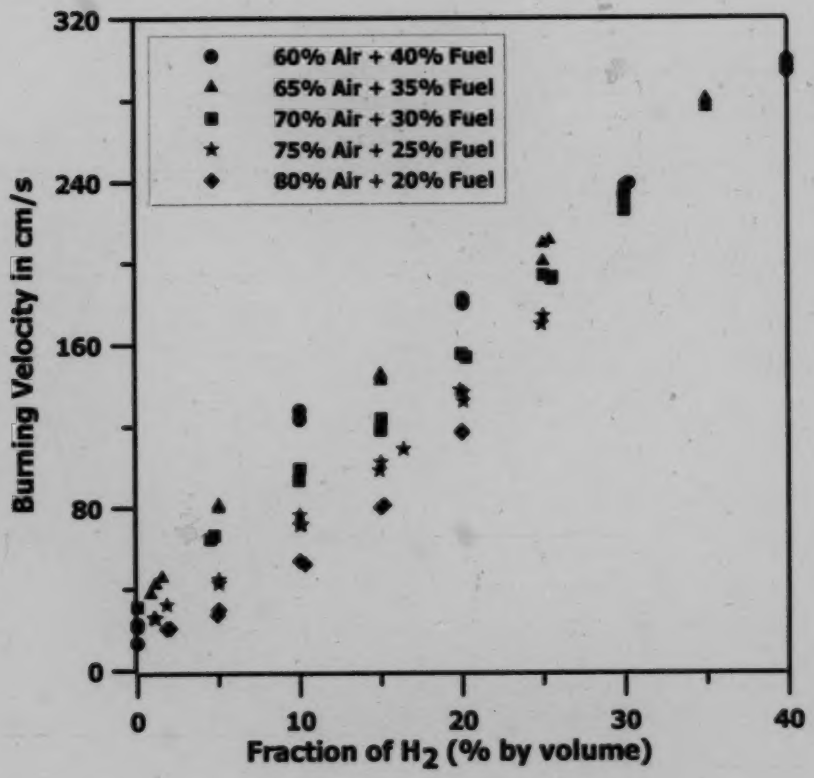


Figure 5.9: Effect of increasing Hydrogen fraction on the burning velocity at different air-fuel ratios

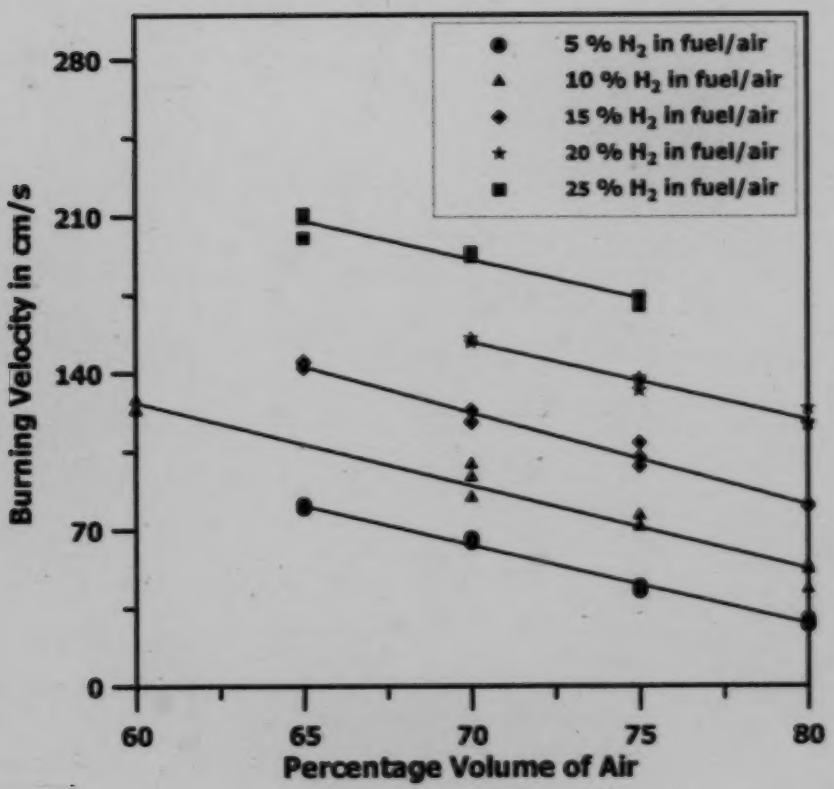


Figure 5.10: Effect of Hydrogen-air volume fraction on the burning velocities Carbon monoxide-Hydrogen

CHAPTER 6

Conclusions and Future Work

6.1 Conclusions

This chapter provides the major conclusions drawn from the study. The literature survey showed a dearth in studies of methane-air-diluent mixtures, methane-air-diluent-reformer gas (RG) mixtures and a varying fraction of CO-H_2-air mixtures. The first part of the study deals with the determination of the laminar burning velocities of various mixtures of methane, air, Simulated Exhaust Gas (SEG) and RG. A cubical combustion chamber was used with all the experiments done at an initial temperature of 298 K and an initial pressure of 1 atm. The main objective of the study firstly is determining the rate of decrease in the burning velocity of methane-air when SEG is added and secondly determining the amount of Reformer Gas required to be introduced in the mixture to rise the burning velocity back to the undiluted levels. The results obtained with SEG addition agreed fairly well with the previous studies.

The burning velocity of the stoichiometric methane-air mixture was found to be 34.9 cm/s. The burning velocity gradually decreased as SEG was added to the mixture. When SEG replaced 4 % of the methane-air the burning velocity dropped to 28 cm/s. This trend continued, as 16 % $\mathcal{V}_{SEG}$ resulted in a burning velocity of 16 cm/s. The change in the burning velocity decreases slightly with higher SEG volume fractions, 20 % $\mathcal{V}_{SEG}$ gave a burning velocity of 13 cm/s and the mixture failed to ignite at higher SEG volume fractions. It was also noted that as the initial pressure was increased to 2 atm, it was possible to replace up to about 30 % of methane-air with SEG. If the SEG was increased any higher the mixture stopped burning.

The percentage by volume of RG required to raise the burning velocity back to undiluted levels varies with the percentage of SEG used. At 4 % $\mathcal{V}_{SEG}$ level, 14 % $\mathcal{V}_{RG}$ was required. This trend continues linearly to an $\mathcal{V}_{SEG}$ fraction of 20 % requiring 42 % $\mathcal{V}_{RG}$ to restore the original undiluted burning velocity.

It was shown in the first part of the study that reformer gases can be used to increase the burning velocity of methane-air-SEG mixtures. Then the knowledge of burning velocity of the reformer gas mixtures assumes paramount importance if the mixture is to be used in any kind of combustion system, since almost all the combustion properties of gas mixtures are dependent on the burning velocity. Hence the need to find the burning velocity of different CO and H_2 fractions.

The purpose of the final part of this study was to measure the laminar burn-

ing velocities of a varied range of CO-H_2-air mixtures. The laminar burning velocities of mixtures of H_2-air and CO-H_2-air have been measured in a cubical combustion chamber with initial temperature at 298 K and initial pressure at 1 atm. The volume fraction of air was varied from 60-80 % in increments of 5, the equivalence ratio varied from 0.6 to 1.6 and the fraction of H_2 in fuel from 0-100 %. These data are expected to be useful for practical as well as modelling purposes.

Burning velocity of stoichiometric H_2 from the Lewis and von Elbe model was found to be 230 cm/s and that from the MTEM was found to be 196.6 cm/s. The burning velocity gradually decreases as CO is added to the mixture. When all of the H_2 in the fuel is replaced by CO in the CO-H_2 mixture the burning velocity drops to around 30 cm/s (Lewis and von Elbe) and 24 cm/s (MTEM).

The burning velocity at an equivalence ratio of 1 for different $\mathcal{V}_H$ was also measured. The burning velocity increases from about 31 cm/s for 0 % $\mathcal{V}_H$ to about 120 cm/s for 15 % $\mathcal{V}_H$ and about 230 cm/s for 30 % $\mathcal{V}_H$. The burning velocity obtained from the MTEM model was found to be lower than that obtained from the Lewis and von Elbe model.

6.2 Future Work and Recommendations

The direction of future work in this area would be the determination of turbulent burning velocities. Since the existing equipment allows the creation of

turbulence in the cubical combustion chamber, with a few modifications to the data acquisition program the turbulent burning velocities can be determined fairly easily. The turbulent burning velocities may prove more useful in simulating the engine conditions in an automobile. High speed or schlieren photography could also be employed to find the burning velocities by flame growth visualization. This will be very useful in finding the burning velocities at the early stages of combustion.

Experiments can also be performed at higher initial pressure and temperature, to measure the pressure-temperature dependency of the laminar burning velocity of methane-air-diluent mixtures. There hasn't been a lot of work done on that subject. Construction of a spherical combustion chamber which could withstand higher pressures could be undertaken, so that the shape effects are minimized or delayed. The precise sensor pressure transducer could be offset to the reading of the validyne pressure transducer at the start of the experiment as the validyne pressure transducer is more accurate at the low pressures.

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APPENDIX A

EGR SIMULATION

The chemical equation for stoichiometric combustion of methane and n-octane are given below:

$$CH_4 + 2\,(O_2 + 3.773\,N_2) \longrightarrow CO_2 + 2\,H_2O + 7.546\,N_2 \qquad (A.1)$$

$$C_8H_{18} + 12.5\,(O_2 + 3.773N_2) \longrightarrow 8\,CO_2 + 9\,H_2O + 47.1625\,N_2 \qquad (A.2)$$

The combustion products of the stoichiometric combustion are CO_2, N_2 and H_2O. Since it is not practical to add water or steam to the combustion chamber, a mixture of N_2 and CO_2 is used to simulate the combustion products. The specific heats of the mixture is compared to the specific heats of the actual products. This comparison is done in the same range as the unburned gas temperature will vary which is from about 298 K to 388 K; so this range is picked to determine the exact volume percentage of N_2 and CO_2 needed to simulate the exhaust gases. Figure A.1 shows the variation of the specific heat of various mixtures of N_2 and CO_2 with increasing unburned gas temperatures. It also shows the variation of specific heat of the combustion products

of stoichiometric methane and n-octane combustion. As seen in the Figure A.1 the specific heat varies from about 30.75 kJ/kmol/K at about 300 K to about 31.25 kJ/kmol/K at about 390 K. The mixture of N_2 and CO_2 whose specific heats match this would be 81.5% N_2 and 18.5% CO_2 whose specific heat varies from about 30.6 kJ/kmol/K at 300 K to about 31.3 kJ/kmol/K at 390 K.

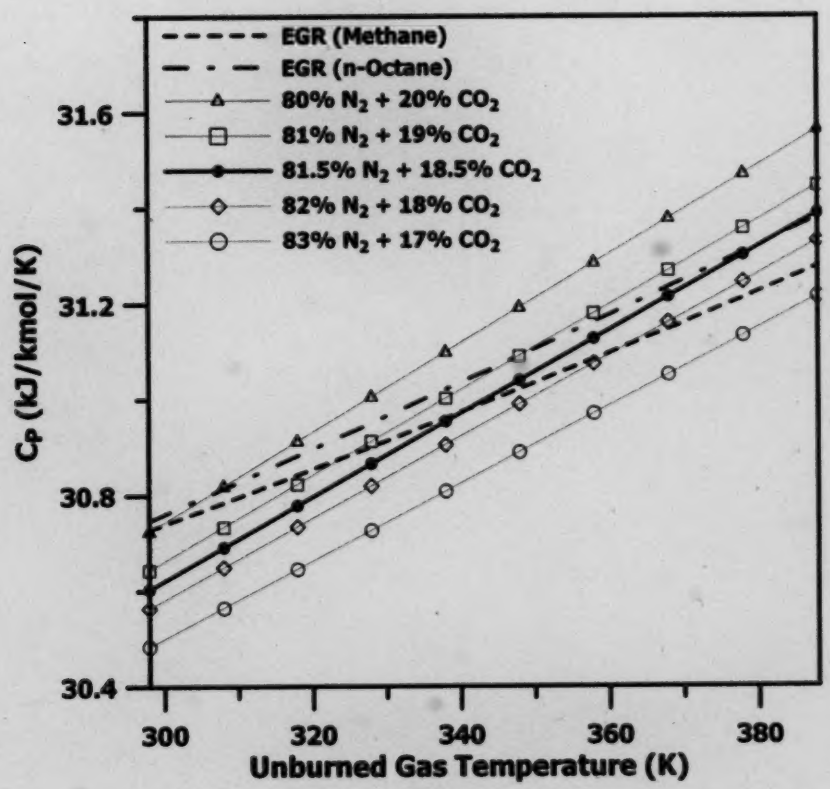

Figure A.1: The unburned gas temperatures of combustion products of methane, n-octane and simulated mixture of N_2 and CO_2 plotted against Specific Heats

APPENDIX B

CALIBRATION OF PRESSURE TRANSDUCERS

This section explains the calibration of the pressure transducers used in the experiments. As explained earlier the main pressure transducer is a Precise Sensor Model 7820 using a four active arm bonded strain gage. Its full range is absolute vacuum to 250 PSI. Its repeatability is at 0.08 % FSO. Its resonance frequency is 22 kHz which is a lot higher than the frequency at which data is collected 5 kHz . The specified manufacturer's output signal tolerance is ± 1 % FSO. The calibration is done with a dead weight tester and a OMEGA Digital pressure indicator Model PCL-601. The atmospheric pressure during the calibration was 705 mm of Hg. The calibration curve is given in Figure B.1.

The two validyne pressure transducers are calibrated using the OMEGA Digital pressure indicator Model PCL-601. They have a range of 0 to 20 PSI and accurate to ± 0.5 % FSO. Their calibration curves are given in Figures B.2 and B.3.

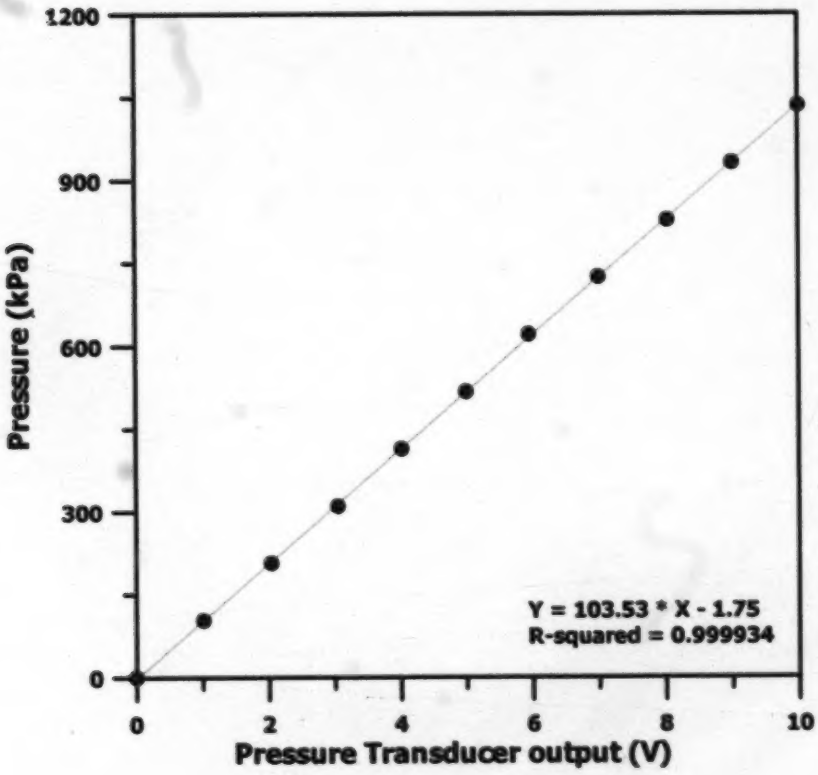

Figure B.1: Calibration curve for the Precise Sensor model 7820 pressure transducer

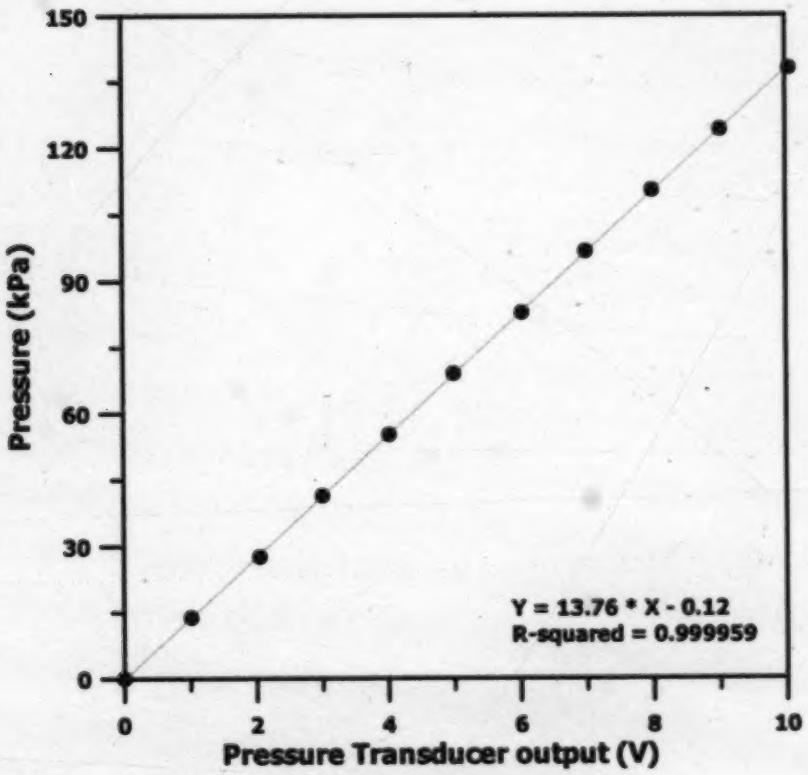

Figure B.2: Calibration curve for the validyne pressure transducer A (Chamber)

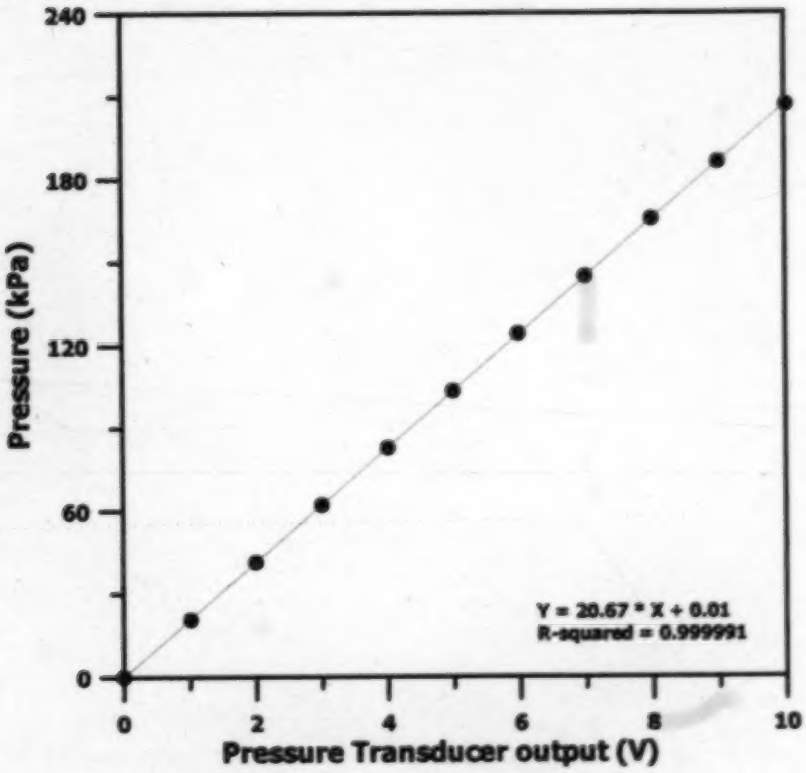

Figure B.3: Calibration curve for the validyne pressure transducer B (Manifold)

APPENDIX C

EXPERIMENTS AT 2 ATM

A few experiments were performed at an initial condition of 2 atm. Since the maximum $\mathcal{V}_{EGR}$ that could burn with methane-air was 22 % at an initial condition of 1 atm, experiments were performed from 24 % at 2 atm. It was found that the mixture could burn upto around 30 % $\mathcal{V}_{EGR}$. But at 30 % $\mathcal{V}_{EGR}$ only gases in the top of the combustion chamber above the electrodes ignited and a normal pressure trace could not be obtained. Experiments below 22 % EG were performed but the maximum pressure exceeded 12 atm and damaged the data acquisition system.

Raw pressure time series for experiments with an initial pressure of 2 atm are shown in Figure C.1 for a range of EGR/fuel mixtures. It can be noted that the mixture is stoichiometric while dilution varies from 24 % $\mathcal{V}_{EGR}$ to 30 % $\mathcal{V}_{EGR}$. The peak pressure attained in the combustion reaction gradually decreases as the percentage $\mathcal{V}_{EGR}$ is increased (Figure C.2). The peak pressure varies from 910 kPa at 24 % $\mathcal{V}_{EGR}$ to 350 kPa at 30 % $\mathcal{V}_{EGR}$. In Figure C.3 the time for the reaction to attain peak pressure is plotted against the fraction of

$\mathcal{V}_{EGR}$. The reaction time increases as the percentage of $\mathcal{V}_{EGR}$ goes up, indicating that the burning becomes slower as more EGR is added to the mixture.

It is shown in Figure C.4, the burning velocity with $P_i = 2\,atm$ gradually decreases with $\mathcal{V}_{EGR}$ addition. The burning velocity hovers around 7 cm/s for 24 % $\mathcal{V}_{EGR}$ and decreases to around 6.2 cm/s for 26 % $\mathcal{V}_{EGR}$ and to 5.7 cm/s at an $\mathcal{V}_{EGR}$ of 28 %. So from this we can infer that as the initial pressure is increased the amount of $\mathcal{V}_{EGR}$ that can be used can also be increased. This will prove to be helpful in engines where the pressure at which the combustion occurs is higher.

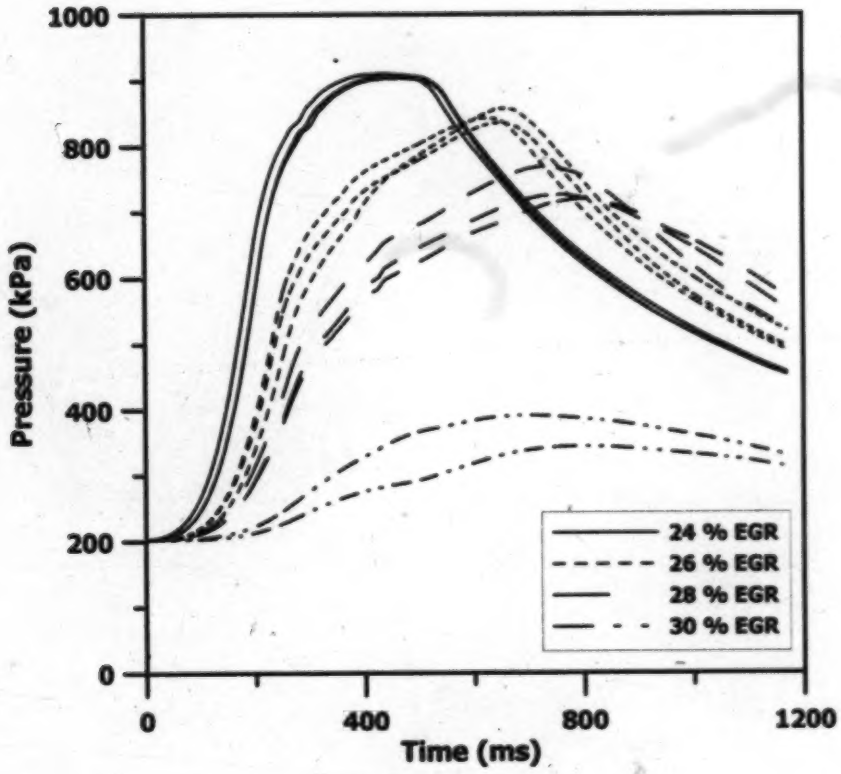

Figure C.1: Raw pressure data plotted against time for different percentage by volume of EGR; $P_i = 2\,atm$

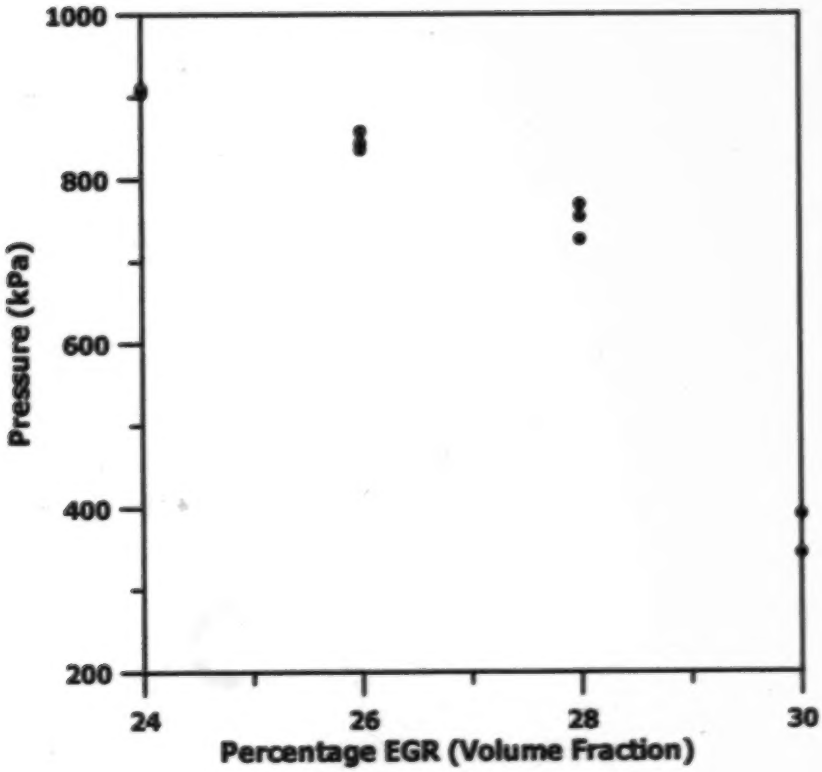

Figure C.2: Effect of increasing $\mathcal{V}_{EGR}$ on Peak Combustion Pressure; $P_i = 2\,atm$

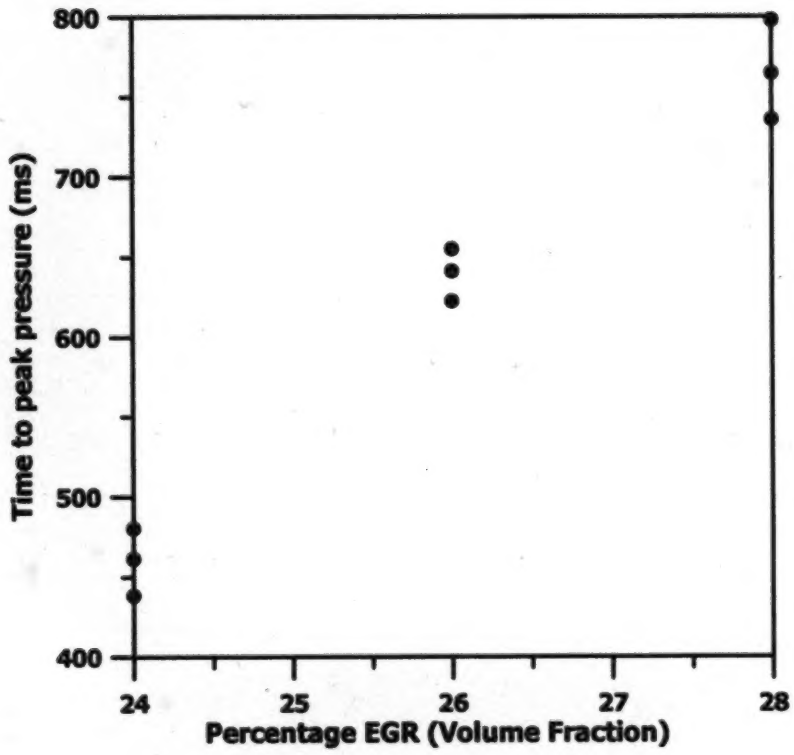

Figure C.3: Effect of increasing $\mathcal{V}_{\text{EGR}}$ on Time to attain Peak Combustion Pressure; $P_i = 2\,\text{atm}$

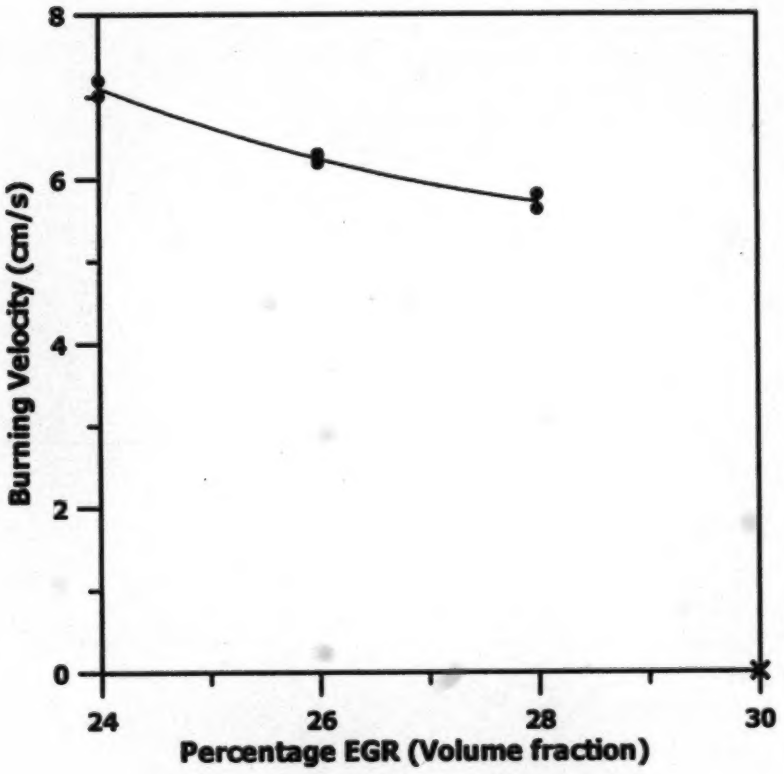

Figure C.4: The decrease in burning velocity with $\mathcal{V}_{\text{EGR}}$ addition; $P_i = 2\,\text{atm}$

APPENDIX D

ERROR ANALYSIS

D.1 Selection of Burning Velocity Data

In spite of all precautions taken to avoid any kind of errors in experiments, there will be uncertainties due to precision of equipments used, human lapse or random errors which arise as a result of noise due to electrical or electronic fluctuations. In the experiments done for this study the human lapse and random errors are countered by neglecting the results which falls out of range. When Chauvenet's Criterion was applied to the data that has been used for discussion and results in the study all the points conformed to it.

D.1.1 Chauvenet's Criterion

Chauvenet's Criterion states that a reading may be rejected if the probability of obtaining the particular deviation from the mean is less than $\frac{1}{2n}$, where n is the number of data [70].

For example, say the burning velocity obtained for stoichiometric methane-air mixtures are 35 cm/s, 34.3 cm/s, 35.3 cm/s, 34.5 cm/s, 34.9 cm/s and 29 cm/s. So we can see from the values of S_u given above that one of the values (No.6 - 29 cm/s) is conspicuously small when compared to the other values, this might be because of either random errors due to noise or due to human lapse in mixing the right proportions of fuels, but there is no proof pertaining to the fact that those might be the causes for the abnormality. Hence we apply Chauvenet's criterion. The mean of the values is 33.83 cm/s and the standard deviation is 2.4.

The difference between the doubtful value and the mean is 4.78 which is 2.01 S.D, which is higher than the allowed 1.73 S.D by Chauvenet's criterion; value as given in Table 3.5, Page 74 of Experimental Methods for Engineers [70]. So this value can be rejected. The Chauvenet's criterion was applied to all the values in this study and all of the values were within the acceptable range.

D.1.2 Pressure Uncertainty

The uncertainty due to the instrument accuracy in this study could very well be blamed on just the pressure transducers, there will be errors measuring the pressure trace after combustion and there will be errors measuring the partial pressures before combustion. As stated earlier the uncertainty in the pressure measurement of the Precise Sensor transducer from which we obtain all the pressure traces is about 1%.

When the standard deviation of the values for the burning velocity raised to the undiluted levels at 34.24 cm/s were calculated it was found that of 1.3 cm/s at 95 % confidence level. When the burning velocity values of stoichiometric methane-air is calculated this uncertainty in the pressure measurement is translated to an uncertainty in the burning velocity. As explained in Experimental Methods for Engineers [70] we could say the uncertainty in the result i.e., the burning velocity is the maximum error in any parameter i.e., pressure used to calculate the result. So when the maximum error possible in the pressure traces are plugged into the values it varies the resulting velocity by $\pm 1.5\%$, which for a burning velocity value of 35.07 cm/s is ± 0.5 cm/s.

In the case of the validyne pressure transducer the error is about $\pm 0.5\%$ due to instrument uncertainty. This translates to an error in the percentage of gases which are added to the combustion chamber. Since the volume percentage of gases is a direct product of the partial pressures this error translates directly to the percentage volume of the gases.

APPENDIX E

PROGRAMS FOR BURNING VELOCITY CALCULATION

Data.m

```
% DATA_labview_F
% August 2003 Senthil Ponnusamy
% July 2002   Panfeng Han
% June 2002 Senthil Ponnusamy
% May 2002 Panfeng Han
% -------
% Substitute for 4CD16G.BAS & 4CHPLT.BAS
% 1992 & 1993 DSK TING
%
% This program reads data from a EXCEL file obtained from
% Labview program D:\research\program\Laminar.vi
% and then changes it to pressure..
%
% It saves pressure from spark to max
% SAMPLE RATE and STANDARD PRESSURE should be checked before
% the program is run

   %%%%%%%%%%%%%%%%%%%% File reading %%%%%%%%%%%%%%%%%%%%

cd('d:\Multizone\Voltage\'); % This folder should be the initial data from Labview
d = dir('d:\Multizone\Voltage\');
str = {d.name};
[s,g] = listdlg('PromptString','Select a file:',...
            'SelectionMode','single',...
            'ListString',str);   % Open file

 file=str{s};
 fid=fopen(file,'r');

   if fid==-1
      errordlg(' The file could not be opened!');
   end

   % Read file
   data=xlsread(file);

   % Close file
   fclose(fid);
   cd('d:\Multizone\');

   [row,col]=size(data);

   % save every column as a varible
   colu=data(:,1);    % Column 1 is the pressure trace
```

```
  f = 5000; %sample rate, from Labview program

  dt=1/f;  % sec

  % Input pressure in the room
prompt  = {'Enter room PRESSURE:(exp.708mmHg)'};
title   = 'Input Information';
lines   = 1;
def     = {'700.9'};
answer  = inputdlg(prompt,title,lines,def);

 Patm = 101325/760*str2double(answer{1});  % room pressure  Pa
% fprintf('the room atmosphere pressure is %5.2f Pa \n',Patm);
 p=15*6894.75*colu+Patm; % convert voltage to pressure Pa

 Pstand=101325;  % 1 Standard Atmosphere Pressure

% Vol=(Pstand-Patm)/15/6894.73  % voltage corresponds to Pinit

% colu=roundn(colu,-3); % round voltage to 10^(-3) digs


% I is a vectore of indictes of beginning elements of colu1
 % I=find(colu==roundn(Vol,-3)); % Pinit is NOT room pressure
 % I=find(colu1==0);          % Pinit is room pressure

% if isempty(I)==1 % voltage corresponding to Pinit cannot be found
  %   Vol=colu(1); % the 1st value is thought as Pinit
   %  I=find(colu==Vol);
    %end


% indstart=max(I);  % Index of the beginning of the spark (indstart)
%  indstart=55;  % 55 is chosen as roughly present spark point
% indstart =200;
 indstart=35;

  for i=1:row
    if p(i)==max(p);
    indend=i;    % Index of the maximum pressure
    break
    end
  end

% Pressure from spark to maximum, also is saved later
  ptrace=p(indstart:indend);

%%%
```

```
[p_f2]=Pfilter(p_f1,2);
%[p_f2]=SLFILT(p_f1, n, 2);


  %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%% GRAPHS
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%


  button = questdlg('Plot Voltage-Time and Pressure-Time Graphs?',...
    'Continue Operation','Yes','No','Help','No');
  if strcmp(button,'Yes')


subplot(2,1,1)
plot(T,P)
ylabel('Pressure (kPa)')
xlabel('time (ms)')
grid

subplot(2,1,2)
plot(T,p_f2)
ylabel('Pressure (kPa)')
xlabel('time (ms)')
grid

  elseif strcmp(button,'No')
    % Do Nothing
  elseif strcmp(button,'Help')
    disp('Sorry, no help available')
  end



% &&&&&&&&&& OUTPUT FILE &&&&&&&&&&

cd('d:\Multizone\pressure\');
[newfile,newpath] = uiputfile('d:\Multizone\pressure\*.csv','Choose Output File Name');

  cd(newpath);
  fid=fopen(newfile,'w');

  fprintf(fid,'%10.6f\n',p_f2);
  fclose(fid);

cd('d:\ Multizone\')

function BOMB


%     BOMB-A.M  multi-zone thermodynamics equilibrium model calculation
%
%     25-NOV-88     M.D. CHECKEL
%     11-AUG-93     D.S-K. TING
%     AUG-2002      Changed to Matlab based on BOMB-A.BAS
%                   Panfeng Han
%     NOV-2002      Changed for fuel mixtures
%                   Panfeng Han
%
% NOTE:  After any major alteration, update the above list and VERDAT$.
%
% FUEL:   CO, H2, CH4
% DILUENT: CO2, N2
%-------------------------------------------------------------------
```

```
% PROGRAM HISTORY:
% Based on BOMB.BAS by Alun Thomas.
% This program is used in conjunction with the program BP2-92 which uses measured pressure record
% and combines it with the calculated quantities from this program.  For most properties, a simple
% interpolation is used to match measured pressures with corresponding values from this program.
% See BP2-02-1 for more information. This program calculates fates of elements of lean fuel-air
% mixtures at specified starting conditions, burning in a constant volume
% combustion cell.
% **********************************************************
% elements are of equal mass fraction
% elements are of equal initial unburned radius square
% i.e. dr(before ignition)^2 = constant
%**********************************************************
% Thermodynamic properties and methods are used as described in:
%               Rowland S. Benson,
%               'Advanced Engineering Thermodynamics'
%               Pergammon Press, 1977, 2nd Edition
% Mixture properties are used as described in:
%               Y A. Cengel
%               'Thermodynamics An Engineering Approach'
%                3rd Ed, 1998 Chapter 12 Gas Mixtures
% Include common statements and routines, dimension
% Changed the total program again based on BOMB-A

clear all
rmol = 8314.3;          %ideal gas constant in J / kgmol k

% Choose fuel(s)
d={'CO', 'H2', 'CH4','C3H8','CO2','N2'};
[s,g] = listdlg('PromptString','Select Mixtures:',...
                'SelectionMode','multiple',...
                'ListString',d);
   j=1;
for i=s
 FUEL (j)=cellstr(d{i});
j=j+1;
end

% Input the volume/molar fractions of fuel mixtues
prompt  = {'Enter volume fraction of CO, eg(9)',...
           'Enter volume fraction of H2, eg(5)',...
           'Enter volume fraction of CH4,eg(9)',...
           'Enter volume fraction of C3H8,eg(5)'};

title  = 'FUELS';
lines  = 1;
def    = {'0','0','0','0'};
answer = inputdlg(prompt,title,lines,def);

Fco   = str2double(answer(1))/100;
Fh2   = str2double(answer(2))/100;
Fch4  = str2double(answer(3))/100;
Fc3h8 = str2double(answer(4))/100;

disp('----FUEL---------')
fprintf('fraction of CO %5.5f \n',Fco);
fprintf('fraction of H2 %5.5f \n',Fh2);
fprintf('fraction of CH4 %5.5f \n',Fch4);
fprintf('fraction of C3H8 %5.5f \n',Fc3h8);
prompt  = {'Enter volume fraction of CO2, eg(10)',...
           'Enter volume fraction of N2, eg(5)'};

title  = 'DILUENTS';
lines  = 1;
```

```
def    = {','};
answer = inputdlg(prompt,title,lines,def);

% Volume / molar fraction of fuels
% They are all changed to percentage fraction here
% and will be used in later all subroutines.
Fco2   = str2double(answer(1))/100;
Fn2    = str2double(answer(2))/100;
Fair   = 1-Fch4-Fco-Fh2-Fc3h8-Fco2-Fn2;

disp('----DILUENT---------')
fprintf('fraction of CO2 %5.5f \n',Fco2);
fprintf('fraction of N2 %5.5f \n',Fn2);
fprintf('fraction of AIR %5.5f \n',Fair);
  disp('--------------------')

perc=[Fco Fh2 Fch4 Fc3h8 Fco2 Fn2 Fair];

  [CC, CW, I, W, IC]=EQCONST;
  [Equiv]=Equiv2 (perc);
  Vtot = 0.001882;

%-------------------------------------------------------------
% Enter initial conditions to work on.
% Input pressure and temperature in the room
prompt = {'Enter initial PRESSURE:(exp.101325Pa)',...
          'Enter initial TEMPETURE: (exp. 24C)'};
title  = 'Input Information';
lines  = 1;
def    = {'101325','23'};
answer = inputdlg(prompt,title,lines,def);

 Pinit = str2double(answer{1});            % pre-combustion pressure in Pa
 Tinit = 273.15+str2double(answer{2});     % pre-combustion temperature in K

% INPUTSECTION:
% Echo back some of the initial parameters for the user

  Rbomb = (0.75 * Vtot / pi) ^ (1 / 3);
  fprintf('Initial Temperature is %5.2f K \n', Tinit);
  fprintf('Initial Pressure is %5.0f Pa \n',  Pinit);
  fprintf('Equivalence ratio is %5.3f\n',Equiv);

 Ntot = 1500;   %1500 elements
 Nb   = 500;    %500 elements to burn

[FCA,FHA,FOA,FMW,mOXY,MF,molR,mN2,MWR,R]=REACTPROP2(Equiv,FUEL,perc);

% MPR = kmol of fuel / element
% MWR = molar mass of reactant mixture (kg/kmol)

  [k]=fngamR1(Tinit,FUEL,perc);
  GMR = k;
  Mass = MWR * Pinit * Vtot / rmol / Tinit;
  fprintf( 'Initial mass is: %5.5f kg, \nMWR=%5.3f kg/kmol \n', Mass,MWR);

  totWRK=0;   % Initial value of total work done
  SUMVBA = 0; % Initial value of the burnt volume
  Pe=Pinit;

h = waitbar(0,'Calculating Main Loop...');

  for I = 1 : Nb
```

```
    dVRatio=(I^(3/2)-(I-1)^(3/2))/Ntot^(3/2);
    MPR = Mass*dVRatio/MWR/molR;
% Pressure before burning element I% is set to Pinit if I%=1 or to Pe,
% the pressure after burning the last element, if I% is greater than 1.
% Pi is the pressure of the element (not to be confused with Pinit)

        Pi=Pe;  % instead of IF loop in Qbasic

% Estimate P after next element burns.
% Pe is the end pressure for the element that is just a guess now.

        Pe = Pi + Equiv / Ntot^(3/2) * Pinit;

% Flag is set to 0 = > that P is only a guess.

        ifLP = 0;

% T reactants and GAMMA reactants are evaluated for this Pi.

        Tr = Tinit * (Pi / Pinit) ^ ((GMR - 1) / GMR);

    [k]=fngamR1(Tr,FUEL_perc);
    GMR = k;

%CALCVOLUMES:
  CALCVOLUMES=1;  % CALCVOLUMES is a flag, 1 continue and 0 stop
  while CALCVOLUMES==1

% This section now calculates the volume of the remaining unburnts before and % after combustion of
% this element. The work done to compress the unburnts is % evaluated and then a loop adds the
% work done to compress each previously % burned element.!if the correct pressure has been
% selected, the work done on all elements will equal the work done by the burning element during its
% combustion and expansion...ie it will match the difference between internal energy of that element
% before and after combustion. When this happens, the selected pressure will be the correct pressure
% after this element burns.
% if the correct pressure is guessed, the sum of the volumes will equal the total volume.
% VUB is the total volume of all the unburnt gases in m^3 BEFORE combustion
% of the Ith element (excludes the Ith element).
% VUA is the total volume of all the unburnt gases in m^3 AFTER combustion
% of the Ith element.

    VuRatio = 1-(I/Ntot)^(3/2);
        VUB = Vtot*VuRatio*(Pinit / Pi) ^ (1 / GMR);
    VUA = VUB * (Pi / Pe) ^ (1 / GMR);

% Calculate the work of compression  (VUB -> VUA) on unburned elements in J.
% negative => work done by the burning element
        WU = -(Pe * VUA - Pi * VUB) / (1 - GMR);

% Volume sum and work sum are set equal to the volume of unburned gas and work done to compress
% the unburned gas in m^3 and joules respectively.

        SUMW = WU;

% if there are previously burned elements, calculate the volume of each before and after compression
% to new pressure, Pe. then calculate the work done to compress each one and add it to the work sum
% done by the burning element.

% VB is the volume of the Jth element before compression.
% VA is the volume of the Jth element after compression.
% WB is the compression work of the Jth element in Joules.
% negative => work done By the burning element
% SUMVBA is the volume of the burnt gases after combustion of element I.
```

```
% STORE(J,3) is the volume of the Jth element after combustion.
% STORE(J,1) is the pressure of the Jth element after combustion.
% STORE(J,9) is the specific heat ratio of products in element J. (=FNGAMP(T))

        if I > 1
   SUMVBA = 0;
          for J = 1:( I - 1)
                VB = STORE(J, 4) * (STORE(J, 1) / Pi) ^ (1 / STORE(J, 10));
                VA = STORE(J, 4) * (STORE(J, 1) / Pe) ^ (1 / STORE(J, 10));
                WB = -(Pe * VA - Pi * VB) / (1 - STORE(J, 10));
   % negative => work done by the burning element
                SUMVBA = SUMVBA + VA;
                SUMW = SUMW + WB;
        end
   end
        SUMV = VUA + SUMVBA;
        SUMW2 = SUMW;

% Use subroutine FLAME to find the temperature of combustion of the burning element knowing its
% starting conditions and work output, SUMW.

        works = SUMW / MPR;   % J/(kmol of fuel/element)

        [T, MWR, MWP,molP,M]=FLAME2 (1,0,works,Pe,Tr,Equiv,FUEL,perc);

  % T=abs(T);

% Calculate the volume this element would have if it burned to temperature T at pressure Pe. (MOLP is
% number of moles of products per mole of fuel, MOLR is moles of reactants per mole of fuel.  Hence
% VE is in m^3 like V).

        VE = Vtot*dVRatio* Pinit / Pe * T / Tinit * molP / molR;

% Compare this with volume left over from unburned gas and all previous burned elements at this
% pressure, Pe.

        ErV = VE - (Vtot - SUMV);

% if the error is greater than .1%, then make a new estimate of pressure and go back to try again.

        ErrLim = VE * 0.0001;
   if Pi<1.1*Pinit
     ErrLim=VE*0.001;
   elseif Pi>2.5*Pinit
     ErrLim=VE*0.0002;
   end
        if abs(ErV) > ErrLim

% ifLP is a flag that determines whether a previous estimate has been made. if it has,
% Extrapolate/interpolate to get a new estimate. Otherwise, simply make a small step in pressure.

          if ifLP > 0
                Pe3 = (Pe * ERV1 - Pe1 * ErV) / (ERV1 - ErV);
                Pe1 = Pe;
                Pe = Pe3;
     else
                Pe1 = Pe;
                ifLP = 1;
                if ErV > 0
                      Pe = Pi + 1.2 * (Pe - Pi);
       else
                      Pe = Pe + (Pe - Pi) / 1.2;
       end
     end
```

```
% Having established this estimate for pressure after combustion, record the current volume error and
% go back to re-calculate the volumes and compression work with the new pressure value.

            ERV1 = ErV;
            CALCVOLUMES=1; % continue to run the while loop
  else % if abs(ErV) <= ErrLim
    CALCVOLUMES=0; %stop the while loop
        end  %end if abs(ErV) > ErrLim
   end    %end while  CALCVOLUMES==1

% Calculation of volumes having converged, enter values for the lth element into the storage arrays

        STORE(I, 1) = Pe;    %pressure of element after combustion
        RR(I) = ((Vtot - VUA) / Vtot) ^ (1 / 3);
        STORE(I, 2) = RR(I);   %relative flame radius after element i burns
      orR(I)=(I/Ntot);       %relative radius before ignition
        STORE(I,3)  = (I/Ntot)^(3/2); % mass fraction burnt

  STORE(I, 4) = VE ;   %volume of elmment after combustion
        STORE(I, 5) = VUB;   %volume of unburned before element has burned
        STORE(I, 6) = VUA;   %volume of unburned after element has burned
        STORE(I, 7) = Tr;      %temperature of the reactants
        STORE(I, 8) = T;       %temperature of element after combustion
  [k]=fngamR1(Tr,FUEL,perc);
  STORE(I, 9) = k;
                                %specific heat ratio of reactants in element #I

        [k]=fngamP(T,M);
  STORE(I, 10) = k;
                                  %specific heat ratio of products in element I%
        STORE(I, 11) = MWP;   %molecular weight of products

% Print out a running listing to let the user know the progress of the calculations that are going on.
%fprintf('%2.0f, %2.0f,P=%5.3f Pa, \n Tb=%5.3f K, r/R=%5.3f \n', i, N, Pe, t, RR);
% The total work done is summed in order to compare this program with STANJAN.  (ie internal energy % change = work
done)

        totWRK = totWRK + SUMW2;

waitbar(I/Nb,h);
end % end for  I = 1 : Nb

fprintf('TOTAL WORK DONE IS %5.5f J/kmol \n', totWRK);
fprintf('\n')

%Prepare the necessary data for writing to data file.
  NR=Nb;
  DD=zeros(NR,7);
  DD(1, 1) = 0;
  DD(1, 2) = Pinit / 1000;  %Pa to kPa
  DD(1, 3) = 0;
  DD(1, 4) = 0;
  DD(1, 5) = Tinit;
  DD(1, 6) = Tinit;
  [k]=fngamR1(Tinit,FUEL,perc);
  DD(1, 7) = k;

  for i = 2 : NR
        DD(i, 1) = i - 1;
        DD(i, 2) = STORE(i - 1, 1) / 1000;  % Pa to kPa pressure of element after combustion
        DD(i, 3) = STORE(i - 1, 2);         % relative flame radius after element i burns
        DD(i, 4) = STORE(i - 1, 3);         % mass fraction burnt
        DD(i, 5) = STORE(i - 1, 7);         % temperature of the reactants
```

```
            DD(i, 6) = STORE(i - 1, 8);          % temperature of element after combustion
    DD(i, 7) = STORE(i - 1, 9);                  % specific heat ratio of reactants
  end

% Construct #(NR+1) row to save percentage of mixtures and
% equivalent ratio
    DD(NR+1,1)=Equiv;
    DD(NR+1,2)=Fco;
    DD(NR+1,3)=Fh2;
    DD(NR+1,4)=Fch4;
    DD(NR+1,5)=Fco2;
    DD(NR+1,6)=Fn2;
    DD(NR+1,7)=Fair;

cd('d:\Multizone\theory\')

[fname,newpath] = uiputfile('d:\Multizone\theory\*.csv','Choose Output File Name');

file = fopen(fname,'w');  % creat a new file

% Write the data to the file
[n,m] = size(DD);
for i = 1:n
   for j = 1:m
      if j == m
         fprintf(file,'%5.7f,\n',DD(i,j));
      else
         fprintf(file,'%5.7f,',DD(i,j));
end
end
end
fclose(file);    % close the file
cd('d:\Multizone')


function BP2_02


%    Aug-1993   D.S-K. Ting
%    Oct-1992   D.S-K. Ting
%
% BP2-02.m is part 2 of Bomb-M1.m and/or Bomb-R.bas. It based on BP2-93.BAS It works for
% BMOB_A02 and save percentage of mixtures and equivalence ratio

% This program calculates fates of elements of lean fuel-air mixtures at specified starting conditions,
% burning in a constant volume bomb, based on the recorded pressure trace from the bomb. It reads
% results from Bomb-A and then interpolates them to match with the measured pressure results.

% Based on BOMB.BAS per Alun Thomas' BOMB.BAS with corrections re units, etc
% Thermodynamic properties and methods as described in:
%          Rowland S. Benson,
%          "Advanced Engineering Thermodynamics"
%          Pergammon Press, 1977, 2nd Edition
% DD  -- theoretical data  (multi-zone model).
% ED  -- experimental data  (pressure transducer).
% Res  -- resolution obtained from BP2_02.m
%

clear all
  f = 5000; % sample rate, from Labview program
  dt=1000*1/f;  % time interval -- ms
  cd('d:\Multizone\theory');
d = dir('d:\Multizone\theory\');
str = {d.name};
```

```
[s,g] = listdlg('PromptString','Select a theorical data:',...
                'SelectionMode','single',...
                'ListString',str);   % Open file
file=str{s};
fid=fopen(file,'r');

 DD=csvread(file);
      fclose(fid);

[DNR,DNC]=size(DD);

cd('d:\Multizone\pressure');
d = dir('d:\Multizone\pressure\');
str = {d.name};
[s,g] = listdlg('PromptString','Select a experimental data:',...
                'SelectionMode','single',...
                'ListString',str);   % Open file
file=str{s};
 fid=fopen(file,'r');
   if fid==-1
     errordlg(' The file could not be opened!');
   end

   ED=csvread(file);
   fclose(fid);
  cd('d:\Multizone\');

  [NRR,NCC] = size(ED);
  NP=NRR;
  if NP > 1500
     NP = 1500;
  end

  MaxP = 2.2* max(DD(1:DNR-1,2)); % factor is an number according to pressure.
  fprintf('Maximum pressure to analyze =%5.3f kPa\n', MaxP);

  for I = 1: NP-1
    Time(I) = dt*(I-1);    %start at time zero

    if ED(I) > MaxP
            IMAXP = I - 1;        %end point to analysis
            break
   %GOTO TimeS
    end
    end

% This is the start of the main loop where interpolation is done to determine various quantities from a data base file based on
measured pressure.

   Res(1, 1) = Time(1);      % Time in ms.
   Res(1, 2) = DD(1, 2);     % Pressure after combustion of element.
   Res(1, 3) = 0;            % relative radius of flame vs bomb radius
   Res(1, 4) = 0 ;           % mass fraction burned
   Res(1, 5) = DD(1, 5);     % unburned gas temperature after combustion
   Res(1, 6) = DD(2, 6);     % temperature of element after combustion
   Res(1, 7) = DD(1, 7);     % specific heat ratio of reactants

   for I = 1 : IMAXP

% IMAXP decides the dimension of Res. MaxP decides value of IMAXP.
% IMAXP comes from #row of ED

     Res(I, 1) = Time(I);
     Res(I, 2) = ED(I);
```

```
  for J = 2 : DNR-1
        if DD(J, 2) > ED(I)
          INTERP = (ED(I) - DD(J - 1, 2)) / (DD(J, 2) - DD(J - 1, 2));
          for K = 3 : 7
        Res(I, K) = DD(J - 1, K) + (DD(J, K) - DD(J - 1, K)) * INTERP;
        end
   break
        end  % if DD(J, 2) > ED(I)
   end      % for J = 2 : DNR-1
   end      % for I = 2 : IMAXP

 Res(IMAXP+1,:)=DD(DNR,1:7); % percentages of mixtures

fprintf('\n')
cd('d:\Multizone\result\');

    [fname,newpath] = uiputfile('d:\Multizone\result\*.csv','Choose Output File Name');

if findstr(fname,'csv')==isempty(fname)
  errordlg('filename should has csv','wrong file name');
  end

file = fopen(fname,'w');  % creat a new file

[n,m] = size(Res);
for i = 1:n
  for j = 1:m
    if j == m
      fprintf(file,'%5.7f,\n',Res(i,j));
    else
      fprintf(file,'%5.7f,',Res(i,j));
    end
  end
end
fclose(file);
 cd('d:\Multizone')


function BV_02

% BV_02
% -----
%
% Aug-1993  DSK TING
%
% This program calculates burning velocities from output produced by BP2_02_1A.m
% It also saves the percentages of mixture

cd('d:\Multizone\result');
d = dir('d:\Multizone\result\');
str = {d.name};
[s,g] = listdlg('PromptString','Select a file:',...
          'SelectionMode','single',...
          'ListString',str);  % Open file
file=str{s};
fid=fopen(file,'r');
  DD=csvread(file);
  fclose(fid);
cd('d:\Multizone\');

[Nrow,Ncol]=size(DD);

 Pinit = DD(1,2);    % pre-combustion pressure in Pa
  Tinit = DD(1,5);    % pre-combustion temperature in K
```

```
Vtot = 0.001882;   %the bomb volume in m^3.  It remains constant.
Rcell = (0.75 * Vtot / pi) ^ (1 / 3);  % m
TimeL=DD(1,1);

Rlast=0;
for i=2:Nrow-1
   Rb(i)=DD(i,3)*Rcell;  % flame radius m
   dVjk=Pinit*DD(i-1,5)*Vtot/Tinit/DD(i-1,2); % flame volume
   dVub=dVjk*(DD(i,4)-DD(i-1,4));
   time(i)=DD(i,1);
   dt=(time(i)-TimeL)*0.001;  %convert ms to s
   Rflame=sqrt((Rlast^2+Rb(i)^2)/2);
   deltaV=4/3*pi*Rflame^3+dVub;
   if deltaV < 0
   Ri=0;
   else
      Ri=(0.75/pi*deltaV)^(1/3);
   end
    dRi=Ri-Rflame;
   Su(i)=(dRi/dt)*100; %convert m/s to cm/s
   GRate(i)=((Rb(i)-Rlast)/dt)*100; %convert m/s to cm/s
   Rlast=Rb(i);
   TimeL=time(i);
   XRb(i)=Rb(i)*1000;  % convert m to mm
end
flag=1;   % keep it as 1 to save postive results only
if flag==0% flag=0 to save all results
MD(:,1)='time';
MD(:,2)=DD(1:Nrow-1,2);    % pressure
MD(:,3)=XRb';                % radius of flame mm
MD(:,4)=Su';                 % burning velocity  cm/s
MD(:,5)=DD(1:Nrow-1,5);    % unburnt temperature K
MD(:,6)=DD(1:Nrow-1,7);    % specific heat ratio of reactants
MD(:,7)=DD(1:Nrow-1,4);    % mass fraction

elseif flag==1
Ptrace=DD(1:Nrow-1,2);  % pressure trace
T=DD(1:Nrow-1,5);       % unburned temperature
Gam=DD(1:Nrow-1,7);   % specific heat ratio of reactants
Time=DD(1:Nrow-1,1);   % time series
I=find(Su>0);
su=Su(I)';
p=Ptrace(I); % corresponding pressure
rb=XRb(I)';
Tu=T(I);
k=Gam(I);
time=Time(I);

MD(:,1)=p;    % pressure
MD(:,2)=rb;   % radius of flame mm
MD(:,3)=su;   % burning velocity  cm/s
MD(:,4)=Tu;   % unburnt temperature K
MD(:,5)=k;    % specific heat ratio of reactants

[a,b]=size(MD);
MD((a+1):(a+2),1:b)=zeros(2,b);
MD(a+1,1:b)=DD(Nrow,1:b);
MD(a+2,1:7-b)=DD(Nrow,6:7);
end
fprintf('\n')
cd('d:\Multizone\velocity');


[fname,newpath] = uiputfile('d:\Multizone\velocity\*.csv','Choose Output File Name');
```

```
  if findstr(fname,'csv')==isempty(fname)
  errordlg('filename should has csv','wrong file name');
  end

file = fopen(fname,'w');  % creat a new file

[n,m] = size(MD);
for i = 1:n
   for j = 1:m
      if j == m
         fprintf(file,'%5.6f,\n',MD(i,j));
      else
         fprintf(file,'%5.6f,',MD(i,j));
      end
   end
end
fclose(file);          % close the file
cd('d:\Multizone')


function plot_relation2

% Senthil Ponnusamy April 2003
% Panfeng Han Feb 2003
% Based on plot_relation
% by Jacob Komar, August 7, 2002
% This function plots the results of curve fitting. It calculates curve fit and confidence interval.
% Su from (1.05-2.2) is filtered, and from (1.05-2.2) is curve fitted. After 68% confidence interval
% considered, final curve fit includes (1~2.2).
% The idea of analysis of data comes from
% Experimental Methods for Engineers
% J.P.Holman, 7th Edtion 2001

Patm=101.325;

cd('d:\Multizone\velocity');
d=dir('d:\Multizone\velocity');
str = {d.name};
[s,g] = listdlg('PromptString','Select a file:',...
            'SelectionMode','single',...
            'ListString',str);  % Open file

 %file=str{s};
 fid=fopen(file,'r');

   if fid==-1
      errordlg(' The file could not be opened!');
   end
DD=csvread(file);
  fclose(fid);

[Nrow,Ncol]=size(DD);

cd('d:\Multizone');

    Perc=[DD(Nrow-1,1:5) DD(Nrow,1:5)];
    Equiv=Perc(1);
    P=DD(1:Nrow-2,1);   % pressure
    Rb=DD(1:Nrow-2,2);  % flame radius
    Su=DD(1:Nrow-2,3);  % burning velocity
    Tu=DD(1:Nrow-2,4);  % unburnt temperature
    gam=DD(1:Nrow-2,5);  % specific heat ratio of reactants

      r = find(P>(2.2*Patm));
```

```
    rmin=min(r);
    if isempty(rmin)==1
      rmin=length(P);
    end
b=find(P<1.05*Patm);
bmax=max(b);
p1=P(bmax:rmin);
su1=Su(bmax:rmin);
k1=gam(bmax:rmin);
n=length(su1);
 legendN=sprintf('Equivalent Ratio %.1f ',Equiv);
 plot(p1,su1,'o')
 hold on
 [suf]=Pfilter(su1,3); % filter the burning velocity
 su1=suf';

Pexp=-0.16+0.22*(Equiv-1);
Texp=2.18-0.8*(Equiv-1);
exp=Pexp+Texp*(k1-1)./k1;
px1=(p1/Patm).^exp;
h = polyfit(px1,su1,1);
y1 = polyval(h,px1);
s=sqrt(sum((su1-y1).^2)/(n-1));

% the standard deviation should be less than or equal to 2cm/s
   while s > 2
    d=s*1.96;  % 95% confidence interval
   j=1
   for i=1:n
     if su1(i)>=y1(i)-d & su1(i)<=y1(i)+d
       su2(j)=su1(i);
       p2(j)=P(i);
       k2(j)=gam(i);
       j=j+1;
     end
   end
   n=length(su2);
   % curve fit
   exp2=Pexp+Texp*(k2-1)./k2;
   px2=(p2/Patm).^exp2;
   h=polyfit(px2,su2,1)
   y2=polyval(h,px2);
   s=sqrt(sum((su2-y2).^2)/(n-1));
   plot(p2,su2,'o',p2,y2)
   ylim([30 45])
   pause
   % rename the variables
   gam=k2; P=p2; su1=su2; y1=y2;
   % plot(px2,su2,'o',px2,y2,'-r')
    clear su2 p2 k2 exp2 px2 y2
    end % while s > 2

% Confidence interval for the newest standard deviation the final error should be ≤to 1cm/s
% Justify if points in (1~1.05) includes or not
% ex is extra

   p_ex=P(1:bmax-1);
   k_ex=gam(1:bmax-1);
   su_ex=Su(1:bmax-1);
   exp_ex=Pexp+Texp*(k_ex-1)./k_ex;
   px_ex=(p_ex/Patm).^exp_ex;
   y_ex=h(1)*px_ex+h(2); % 1~1.05 straight line

   d=s*1;   % 68% confidence interval
```

```
plot(p1,su1,'+r',p1,y1)
hold on
% construct the points from (1-2.2)
yf=[y_ex' y1'];
suf=[su_ex' su1'];

m=length(suf);
j=1;
for i=1:m
  if suf(i)>=yf(i)-d & suf(i)<=yf(i)+d
    su2(j)=suf(i);
    p2(j)=P(i);
    k2(j)=gam(i);
    j=j+1;
  end
end
n=length(su2);

% final curve fit
exp2=Pexp+Texp*(k2-1)./k2;
px2=(p2/Patm).^exp2;
h2=polyfit(px2,su2,1);
y2=polyval(h2,px2);
y2_ex=h2(1)*px_ex+h2(2); % 1~1.05 straight line
plot(p2,su2,'sk',p2,y2,'-.k')
hold on
plot(p_ex,su_ex,'>m',p_ex,y2_ex,':k')
ylim([0 20])
xlabel('pressure (kPa)')
ylabel('burning velocity (cm/s)')
legend('original data','filtered data','1st curve fitting','fitted data','2nd curve fitting','data at 1-1.05Patm','extrapolated line',4);

% su--value1 @ 101.325 kPa
% extrapolate gam @ 101.325 kPa

t=min(find(P>=101.325)); % indicate greater than 101.325
u=max(find(P<101.325));  % indicate less than 101.325
if isempty(u)==1
  u=t+1; % extrapolate
  gam=gam(t)+(gam(u)-gam(t))*(101.325-P(t))/(P(u)-P(t));
  else % interpolate
  gam=gam(u)+(gam(t)-gam(u))*(101.325-P(u))/(P(t)-P(u));
end
exp=Pexp+Texp*(gam-1)./gam;
px=1.^exp;
v(1)=h2(1)*px+h2(2)
Equiv;
diluent=Perc(5)+Perc(6);

function [CC, CW, I, W, IC]=EQCONST


%     EQCONST
%     09-DEC-87     M.D. CHECKEL
%     14-SEP-92     Cleaned up, checked and organized.
%                   D.S-K. Ting
%     28-JUNE-2002  Changed to Matlab and combined EQCONST & PROPCOEFF
%
%
%
% This subroutine EQCONST calculates a set of constants used for calculating chemical equilibrium
% coefficients for CO2 dissociation and the Water-Gas reaction. The basic idea is to minimize the gibbs
% free energy in the equilibrium mixture.
% ie ln(Kp) = -{ sum[nu*g(T)]p -sum[nu*g(T)]r } - deltaG298/(rmol*T)
```

```
% where nu is the stoichiometric coefficient for each reactant and product
% and deltaG298 is the difference in gibbs energy of formation at 298 k.

% The subroutine also fills an array with coefficients used in calculating enthalpy and Gibbs function for
% CO, CO2, H2, H2O, N2, O2, and fuel. It also calculates chemical equilibrium constants used for CO2
% and CO2-H2O dissociation reactions.  The IC() array is used for this.
% the data for the coefficients.
% IC() is the coefficient array.

IC= [3.317   3.7697e-4  -3.2208e-8  -2.1945e-12  0 4.63284 -1.13882e8;...          %CO
     3.0959  2.73114e-3 -7.88542e-7 8.66002e-11  0 6.58393 -3.93405e8;...          %CO2
     3.43328 -8.181e-6  9.6699e-8   -1.44392e-11 0 -3.8447 0;...                   %H2
     3.74292 5.65590e-4 4.9524e-8   -1.81802e-11 0 0.96514 -2.39082e8;...          %H2O
     3.34435 2.9426e-4  1.953e-9    -6.5747e-12  0 3.75863 0;...                   %N2
     3.25304 6.5235e-4  -1.49524e-7 1.53897e-11  0 5.71243 0;...                   %O2
     1.13711 1.45532e-2 -2.95876e-6 0.0          0   0.0  -0.90510e8;...          %C3H8
     1.93529 4.96462e-3 -1.24402e-6 1.62497e-10  -8.58611e-15 8.153 -6.69305e7];  %CH4

%  CO2 dissociation:       CO + (1/2) O2 <-> CO2
%  Kco2 = MCO2/(MCO2(MCO*SQR(MO2*PIN/(mp*Pn))
     %            CO          O2          CO2
          CC(1) = IC(1, 1)  + IC(6, 1) / 2 - IC(2, 1);       % 1st
          CC(2) = IC(1, 2)  + IC(6, 2) / 2 - IC(2, 2);       % 2nd
          CC(3) = (IC(1, 3) + IC(6, 3) / 2 - IC(2, 3)) / 2;  % 3rd
          CC(4) = (IC(1, 4) + IC(6, 4) / 2 - IC(2, 4)) / 3;  % 4th
          CC(5) = IC(1, 6)  + IC(6, 6) / 2 - IC(2, 6);       % 5th
          CC(6) = IC(1, 7)  + 0 - IC(2, 7);                  % hoR-hoP


% Water-Gas reaction:     CO + H2O <-> CO2 + H2
% Kwg = MCO2*MH2/(MCO*MH2O)


%              CO2         H2         CO       H2O
          CW(1) = -IC(2, 1)  - IC(3, 1) + IC(1, 1) + IC(4, 1);       % 1st
          CW(2) = -IC(2, 2)  - IC(3, 2) + IC(1, 2) + IC(4, 2);       % 2nd
          CW(3) = (-IC(2, 3) - IC(3, 3) + IC(1, 3) + IC(4, 3)) / 2;  % 3rd
          CW(4) = (-IC(2, 4) - IC(3, 4) + IC(1, 4) + IC(4, 4)) / 3;  % 4th
          CW(5) = -IC(2, 6)  - IC(3, 6) + IC(1, 6) + IC(4, 6);       % 5th
          CW(6) = -IC(2, 7) -      0    + IC(1, 7) + IC(4, 7);       % hoR-hoP

% I() is the alphanumeric name.
% W() is the molecular weight.

% The coefficients and methods of use are described in:
% Rowland S. Benson
% "Advanced Engineering Thermodynamics"
% Pergammon Press, 1977, 2nd Edition
% (eg pg 153, Appendix A)
% Propane is per Benson & Baduah, Int J Mech Eng Educ, Vol 4, No 1, p 93

 I = {'CO', 'CO2', 'H2', 'H2O', 'N2', 'O2', 'C3H8','CH4'};
 W = [28.0134 44.00995 2.016 18.016 28.0155 31.9988 44.09 16.04];
 % P = IC';    % another coefficient for thermodynamic properties


function [k]=fngamR1(T,FUEL,perc)

% Program to calculate k
%                MD CHECKEL        11 DECEMBER, 1987
%                (BASIC)
%                SENTHIL PONNUSAMY    4 JULY, 2002
%                (MATLAB)
```

```
% Read in the data for the property coefficients.
% Data statements are at end of the "main" program.
% Data taken from :  R.S Benson, Advanced Engineering Thermodynamics
%                    2nd Ed,1977. Appendix A
Rmol=8314.3;
[CC, CW, I, W, IC]=EQCONST;
% CO=1, H2=3,C3H8=7, CH4=8 CO2=2 O2=6 N2=5

Fco  = perc(1);
Fh2  = perc(2);
Fch4 = perc(3);
Fc3h8 = perc(4);
Fco2  = perc(5);
Fn2   = perc(6);
Fair  = perc(7);

sumCp=0;

for j=1:length(FUEL)
 switch FUEL{j}
 case {'CO'}
  i=1;
Cp = Fco*Rmol * (IC(i,1) + 2 * IC(i,2) * T + 3 * IC(i,3) * T ^ 2 + 4 * IC(i,4) * T ^ 3 + 5 * IC(i,5) * T ^ 4);
 case {'H2'}
  i=3;
Cp = Fh2*Rmol * (IC(i,1) + 2 * IC(i,2) * T + 3 * IC(i,3) * T ^ 2 + 4 * IC(i,4) * T ^ 3 + 5 * IC(i,5) * T ^ 4);
 case{'C3H8'}
  i=7;
Cp = Fc3h8*Rmol * (IC(i,1) + 2 * IC(i,2) * T + 3 * IC(i,3) * T ^ 2 + 4 * IC(i,4) * T ^ 3 + 5 * IC(i,5) * T ^ 4);
 case{'CH4'}
  i=8;
Cp = Fch4*Rmol * (IC(i,1) + 2 * IC(i,2) * T + 3 * IC(i,3) * T ^ 2 + 4 * IC(i,4) * T ^ 3 + 5 * IC(i,5) * T ^ 4);
 case{'CO2'}
  i=2;
Cp = Fco2*Rmol * (IC(i,1) + 2 * IC(i,2) * T + 3 * IC(i,3) * T ^ 2 + 4 * IC(i,4) * T ^ 3 + 5 * IC(i,5) * T ^ 4);

end
   sumCp=Cp+sumCp;
  end

% N2 and O2 fraction in Air
F_o2  = Fair*0.2095;
F_n2  = Fair*0.7905;

% N2  -- diluent + fraction in air
Cp_n2=(Fn2+F_n2)*Rmol*(IC(5,1) + 2*IC(5,2)*T + 3*IC(5,3)*T ^ 2 + 4*IC(5,4)*T ^ 3 + 5*IC(5,5)*T ^ 4);
% O2  -- fraction in air
Cp_o2=F_o2*Rmol * (IC(6,1) + 2 * IC(6,2) * T + 3 * IC(6,3) * T ^ 2 + 4 * IC(6,4) * T ^ 3 + 5 * IC(6,5) * T ^ 4);
  sumCp=sumCp+Cp_o2+Cp_n2;
  k  = sumCp / (sumCp - Rmol);       %GAMMA(reactants)


function [Equiv]=Equiv(Fco,Fh2,Fch4,Fc3h8,Fair)

% Equiv.m
% Feb-2003  -- Panfeng Han
% Get equivalence ratio for FUEL mixtures
% equiv=sum(+V)/sum(-V)
% V is chemical valence
% For Example: [Equiv,AtoFactual]=Equiv(0.1,0.2,0,0)
% positive valence
Vp=Fco*4+Fh2*1*2+Fch4*(4+4*1)+Fc3h8*(4*3+8*1);
% negative valence
Vn=Fco*2+0.2095*Fair*2*2;
```

```
% Equivalence ratio
Equiv=Vp/Vn;

function [M,molP,MWP,P]=EQCOMP3(PE,T,Equiv,FUEL,perc)

%     EQCOMP1  Equilibrium composition calculation
%     ******
%     09-DEC-87      M.D. CHECKEL
%     14-SEP-92      Cleaned up, checked and organized.
%                    -- D.S-K, Ting
%     JUN-2002       Changed to Matlab
%                    -- Panfeng Han
%
% This subroutine calculates the equilibrium composition of a hydro-carbon + air flame given a
% temperature, T. Additional information is the set of coefficients calculated in the main program for
% the CO2 dissociation and the water-gas reactions which are the only two reactions considered.
% Information is returned as M(I) which are numbers of moles/mole of fuel.
% M(1)=mCO, M(2)=mCO2, M(3)=mH2, M(4)=mH2O, M(5)=mN2, M(6)=mO2
% equation

1*FUEL+a*O2+3.76*a*N2=M(1)*CO+M(2)*CO2+M(3)*H2+M(4)*H2O+M(5)*N2+M(6)*O2
% INPUT PE:      pressure
%     MF:      moles fuel
%     MWR:     mole weight(reactants)
%     FCA:     fuel carbon atoms
%     FHA:     fuel hydrogen atoms
%
% OUTPUT M:      mole number of products
%      molP:    total mole number of products
%      MWP:     mole mass of products
%      P:       coefficients of products
%
% The 6 constants (A1-A6 per Benson and Hfo) are also calculated for the equilibrium product mixture
% and returned as P(1) through P(7).


[FCA,FHA,FOA,FMW,mOXY,MF,molR,mN2,MWR,R]=REACTPROP2(Equiv,FUEL,perc);
[CC, CW, I, W, IC]=EQCONST;

rmol = 8314.3;          %ideal gas constant in J/kgmol.k
PN = 101325;            %standard atmosphere (for Go and So)
M(5) = mN2;
quit = 1; % flag to jump out the loop
K1=1e-10;
if (MF > 0)&(quit == 1)

% L is a flag to sense failure to converge iterative solution starts by
% assuming no CO2 dissociates.

L = 0;
  if Equiv>=1  % rich mixture
  M(2) = mOXY-FCA/2-FHA/2;
  else
  M(2) = FCA;
  end


% IFLAG=0 indicates this is first guess.
          IFLAG = 0;
          if (T > 500) &(quit == 1)

% Calculate equilibrium constants at the current temperature, T.
```

```
        Fco2 = CC(1) * (1 - log(T)) - CC(2) * T - CC(3) * T ^ 2;
        KCO2 = exp(-(Fco2 - CC(4) * T ^ 3 - CC(5) + CC(6) / T / rmol));
        Fwg = CW(1) * (1 - log(T)) - CW(2) * T - CW(3) * T ^ 2;
        KWG = exp(-(Fwg - CW(4) * T ^ 3 - CW(5) + CW(6) / T / rmol));

% Calculate the kgmol of H2O,CO,H2,O2 and the total kgmol based on the assumed CO2.

INCL=1;
      while (INCL==1)&(quit == 1)
    L = L + 1;
        M(4) = FHA / 2 * M(2) / ((FCA  - M(2)) / KWG + M(2));
        M(1) = FCA - M(2);
        M(3) = FHA / 2 - M(4);

% Calculate CO2 "equilibrium constant" of this composition and see how it compares with that already % calculated above.

        M(6) = mOXY - M(2) - M(1) / 2 - M(4) / 2;
molP = sum(M);
KPCO2 = M(1) * sqrt(M(6) * PE /(molP*PN)) /M(2);
ER = KCO2 - KPCO2;

% If error is small, calculate property coefficients.
% Otherwise, make a new estimate of moles CO2.

if (abs(ER) > 0.00001 *KCO2) & (quit == 1)

% First iteration is to assume 1/2 of the CO2 dissociates.

                    if IFLAG == 0
                                EL = ER;
                                ML = M(2);
                                M(2) = 0.5 * FCA;
                                IFLAG = 1;
% Subsequent iterations use geometric interpolation.

    else
                                M1 = (M(2) * EL - ML * ER) / (EL - ER+realmin);
                                if M1 < 0
      M1 = 0.01;    % must have some CO2
      end
                                if M1 > FCA
      M1 = FCA;     % but not more than FCA
      end
      ML = M(2);
                                EL = ER;
                                M(2) = M1;

    end % IFLAG == 0

    if L < 601

      INCL=1;
      else
      % EFAIL to converge again
       INCL=0; % jump out while INCL==1
      quit=1; % continue run if abs(ER) > KCO2 * 0.00001
      end
else % abs(ER) <= 0.00001 *KCO2
   quit = 0;  % jump out the if loop and run PROP
   break
end  % if abs(ER) > KCO2 * 0.00001
      end  % while INCL==1
   elseif T <= 500
```

```
    fprintf('EQCOMP failure: T= %5.2f', T);
    fprintf('\n iterations L= %5.0f\n',L);
                    M(1) = 0;               %mCO
                    M(2) = FCA;             %mCO2
                    M(3) = 0;               %mH2
                    M(4) = FHA / 2;         %mH2O
                    M(6) = mOXY - FCA - FHA/4;  %mO2
                    T = -T;
    quit=0;   % jump out the if loop and immediately run PROP
    end  % if T < 500

else  % if MF <= 0, i.e. no fuel
            M(1) = 0;
                    M(2) = 0;
                    M(3) = 0;
                    M(4) = 0;
                    M(6) = mOXY + FOA;
    end % end of if MF <= 0
M=real(M);
if M(6) < 0
  M(6)=1e-6; % rich mixtue, there must have some oxygen
end
% Evaluate property coefficients for this equilibrium mixture.
% PROP
P=zeros(1,7);
        for I = 1: 7
                for J = 1: 6
                        P(I) = P(I) + M(J) * IC(J, I);
    end
  end

% Calculate the number of moles of product, molP, and the molecular weight
% of the product, MWP.
% W is the molecular weight.

        molP = sum(M);
        MWP = 0;
        for J = 1:6
                MWP = MWP + M(J) * W(J);
  end
        MWP = MWP / molP;



function [Equiv]=Equiv2(perc)

% Equiv.m
% Mar-2003  -- Panfeng Han
% equiv=sum(+V)/sum(-V)
% V is chemical valence
% [O -2] [N 0] [H +1]  [C +4]
%
% as to lean methane-air mixture, if we use this method
% and include the oxygen & carbon in products which correspond
% to stoich as there was no free oxygen in our residual, that
% averages some equiv=1.0 makes it effectively a little less lean
%
% For Example: [Equiv]=Equiv(perc)

Fco  = perc(1);
Fh2  = perc(2);
Fch4 = perc(3);
Fc3h8 = perc(4);
```

```
Fco2  = perc(5);
Fn2   = perc(6);
Fair  = perc(7);

% positive valence
Vp=Fco*4+Fh2*2+Fch4*8+Fc3h8*20+Fco2*4;

% negative valence
Vn=Fco*2+0.2095*Fair*4+Fco2*4;

% Equivalence ratio
Equiv=Vp/Vn;


function [T, MWR, MWP,molP,M]=FLAME2(IND, Q, WORK, PE, TR,Equiv,FUEL,perc)

%     FLAME    Calculating Temperature
%     10-DEC-87      M.D. CHECKEL
%     13-SEP-92      Cleaned up, checked and organized.
%                    D.S-K. Ting
%     JUNE-2002      Changed to Matlab
%                    Panfeng Han
% INPUTS:
%   IND  = 0 for constant pressure, 1 for varying pressure
%   Q    = heat transfer TO the element during combustion
%   W    = work transfer FROM the gas during combustion (=0 if IND=0) (J/element)
%        - the units of Q and W are ( J/(1 kmol fuel + associated air) )
%   PE   = pressure at the end of combustion (Pa)
%   Equiv = stoichiometric ratio (0<S<1) = (F/A)/(F/A)stoic
%   TR   = reactant mixture temperature (K)
%   MPR  = kmol of fuel / element
%   FUEL  = kind of fuel

% OUTPUTS:
%   T    = flame temperature at equilibrium (K)
%   MWR  = molar mass of reactant mixture (kg/kmol)
%   MWP  = molar mass of products mixture (kg/kmol)

% Get the properties and property coefficients of the reactants.
  [FCA,FHA,FOA,FMW,mOXY,MF,molR,mN2,MWR,R]=REACTPROP2(Equiv,FUEL,perc);
  [CC, CW, I, W, IC]=EQCONST;
  rmol = 8314.3;          %ideal gas constant in J/kgmol.k
         PN = 101325;          %standard atmosphere (for Go and So)

% calculate enthalpy of reactants in J/kmol at temperature TR

         x = R(2) * TR + R(3) * TR ^ 2 + R(4) * TR ^ 3 + R(5) * TR ^ 4;
         enthr = rmol * TR * (R(1) + x) + R(7);

% Guess the initial temperature (based on equivalence ratio).

         T = TR + 2200 * Equiv;
  eri=0;  %initial error value
  T1 = 0;
         T3 = 0;
         FLAG = 0;

% Use subroutine EQCOMP to calculate equilibrium composition at temp T.
% Then calculate the work and energy quantities for first law analysis.

GETCOMP=1;
while GETCOMP==1 % GETCOMP is a flag, 1=continue, 0=stop
  [M,molP,MWP,P]=EQCOMP2(PE,T,Equiv,FUEL,perc);
  if T <= 0
```

```
    T = 2000;
    T1 = 0;
          T3 = 0;
            FLAG = 0;
    [M,molP,MWP,P]=EQCOMP2(PE,T,Equiv,FUEL,perc);
    end

% Calculate enthalpy of products in kJ/kgmol at temperature T
          x = P(1) + P(2) * T + P(3) * T ^ 2 + P(4) * T ^ 3 + P(5) * T ^ 4;
          enthp = rmol * T * x + P(7);
          if IND == 0  %constant pressure
                    eri = enthr + Q - enthp;     % mdc 910712: include HEAT
  else
     intr = enthr - molR * TR * rmol; % internal energy
     intp = enthp - molP * T * rmol;
                    eri = intr + Q - WORK - intp;
  end

% Check the "balance" error in the first law of thermodynamics.
% If error is < 1000 J/(1 kmol.fuel + associated air), then T is OK, end.
          if abs(eri) >= 1000
% try new combustion T.
% For the first iteration, just add or subtract 10 K.

if FLAG == 0
    T1 = T;
                    FLAG = 1;
                    if eri < 0
       T = T - 10;
     else
       T = T + 10;
     end
% For later estimates, use geometric interpolation.
else
                    T3 = (T * ET - T1 * eri ) / (ET - eri);
                    T1 = T;
                    T = T3;
                    FLAG = FLAG + 1;
end
          ET = eri;
          GETCOMP=1;

 else  % if abs(eri) < 1000

    GETCOMP=0;
    break  % terminate the program
 end  % end of if abs(eri) >= 1000
 end  % end of while GETCOMP==1

function Lewis_mixture

% Senthil Ponnusamy Jan 2003
% Panfeng Han Jan. 2003
% cleaned and arranged again April 2003

% Based on IN_OUT
% Jacob Komar & Stephane Masson  - July 29, 2002

% This program reads the pressue trace and calculates burning velocity using Lewis Von Elbe model.
% It works for CH4, CO, H2, CO2 & N2
% the sample rate will be 5000/per second from Labview
% STANJAN has to be run early before run this program
```

```
clear all

cd('d:\Multizone\pressure\'); % This folder should be the initial data from Labview
d = dir('d:\Multizone\pressure\');
str = {d.name};
[s,g] = listdlg('PromptString','Select a file:',...
          'SelectionMode','single',...
          'ListString',str);   % Open file
file=str{s};
fid=fopen(file,'r');
  if fid==-1
    errordlg(' The file could not be opened!');
  end
data=csvread(file);
fclose(fid);

cd('d:\Multizone\Comparison');
[row,col]=size(data);

% save every column as a varible
ptrace=data(:,1);    % Column 1 is the pressure trace

% ---------- Initial Condition ----------------

  f = 10000; %sample rate, from Labview program
  dt= 1000/f;  % ms

% Enter initial conditions,-- the room temperature
prompt  = {'Enter room TEMPETURE: (exp. 24)'};
title   = 'Input Information';
lines   = 1;
def     = {'24'}; % Celius degree
answer  = inputdlg(prompt,title,lines,def);
Ti = 273.15+str2double(answer);   % pre-combustion temperature in K
p=ptrace*1000;     % Pa
Pi=p(1);           % atmospher pressure
n=length(p);
t=0:dt:(n-1)*dt;   % creat time array, ms

% Choose fuel(s) to run the program
d={'CO','H2','CH4','C3H8','CO2','N2'};   % FUEL is picked here
[s,g] = listdlg('PromptString','Select Mixtures:',...
          'SelectionMode','multiple',...
          'ListString',d);
   j=1;
for i=s
FUEL(j)=cellstr(d{i}); % now FUEL is a cell
j=j+1;
end

% Input the volume/molar fractions of fuel mixtues
prompt  = {'Enter volume fraction of CO,  eg(10)',...
           'Enter volume fraction of H2,  eg(5)',...
           'Enter volume fraction of CH4, eg(5)',...
           'Enter volume fraction of C3H8,eg(0)'};

title   = 'FUELS';
lines   = 1;
def     = {'0','0','0','0'};
answer  = inputdlg(prompt,title,lines,def);

% Volume-molar fraction of fuels, they are all changed to percentage fraction here and will be used in % later all subroutines.
Fco   = str2double(answer(1))/100;
```

```
Fh2   = str2double(answer(2))/100;
Fch4  = str2double(answer(3))/100;
Fc3h8 = str2double(answer(4))/100;

% Input the volume/molar fractions of diluents
prompt = {'Enter volume fraction of CO2, eg(10)',...
          'Enter volume fraction of N2, eg(5)'};

title  = 'DILUENTS';
lines  = 1;
def    = {'0','0'};
answer = inputdlg(prompt,title,lines,def);

% Volume/molar fraction of fuels
% They are all changed to percentage fraction here and will be used in later all subroutines.
Fco   = str2double(answer(1))/100;
Fn2   = str2double(answer(2))/100;
Fair  = 1-Fch4-Fco-Fh2-Fc3h8-Fco2-Fn2;
perc=[Fco Fh2 Fch4 Fc3h8 Fco2 Fn2 Fair];

% constant specific heat
[gram]=fngamR1(Ti,FUEL,perc);
Vtot=0.001882;          % m^3
Rcell=(3*Vtot/4/pi)^(1/3); % m

% Equivalence ratio
[Equiv]=Equiv2(perc);
fprintf('Equivalence ratio is %5.2f \n',Equiv);
%-------------------------------------------------
% Input the final pressure,i.e., peak pressure
prompt = {'Enter peak pressure, (from STANJAN) eg(732680)'};

title  = 'Pe';
lines  = 1;
def    = {'800000'};
answer = inputdlg(prompt,title,lines,def);
Pe=str2double(answer);

% Lewis Von Elbe Equation
% ------ Tu, Rb & mf ----------
for j=1:n

% unburnt reactant temperature
Tu(j)=Ti*(p(j)/Pi)^((gram-1)/gram);
[gram]=fngamR1(Tu(j),FUEL,perc);

% flame radius
Rb(j)=(1-(p(j)/Pi)^(-1/gram)*(Pe-p(j))/(Pe-Pi))^(1/3)*Rcell; % m

% burned mass fraction
mf(j)=(p(j)-Pi)/(Pe-Pi);
end

clear gram
[gram]=fngamR1(Ti,FUEL,perc);

% ----- su & k ---------
 for i=2:n-1
 T=Ti*(p(i)/Pi)^((gram-1)/gram);  % Unburnt gas temperature
[gram]=fngamR1(T,FUEL,perc);
k(i)=gram;

% Flame Growth Rate
dRb_dt(i)=100*(Rb(i+1)-Rb(i-1))/2/dt; %convert m/s to cm/s
```

```
% dp/dt, dt--0.1ms,
 dp_dt(i)=(p(i+1)-p(i-1))/2/dt; % Pa/ms,
 %  burning velocity
 % Unit: Rcell--m, dt--ms, 1000*Rcell/dt--m/s, 10^5*Rcell/dt--cm/s
su(i)=10^5*Rcell/(3*(Pe-Pi))*dp_dt(i)*(Pi/p(i))^(1/k(i))*(1-((Pe-p(i))/(Pe-Pi))*(Pi/p(i))^(1/k(i)))^(-2/3);

end
dp_dt=dp_dt/1000;  % convert Pa/ms to kPa/ms
rRb=Rb/Rcell; % relative flame radius
Rb=Rb*1000;   % convert m to mm

Flag = 1; % 1 save picked values, 0 save all raw values

if Flag==0
DD(:,1)=t';              % time from spark to peak ms
DD(:,2)=p/1000;          % pressue trace   kPa
DD(:,3)=Rb';             % flame radius   mm
DD(:,4)=rRb';            % relative flame radius
DD(:,5)=[dRb_dt 0]';     % flame growth rate  cm/s
DD(:,6)=[dp_dt 0]';      % pressure growth rate kPa/ms
DD(:,7)=[su 0]';         % burning velocity   cm/s
DD(:,8)=Tu';             % unburnt gas temperature  K
DD(:,9)=mf';             % burnt mass fraction
DD(:,10)=[k 0]';         % specific heat ratio

elseif Flag==1

Ptrace=p(2:n)/1000;
rb=Rb(2:n);
T=Tu(2:n);
% only positive points left to analysis

I=find(su>0);
su1=su(I)';
P1=Ptrace(I); % corresponding pressure
rb1=rb(I)';
Tu1=T(I)';
k1=k(I)';

DD(:,2)=rb1;             % flame radius (mm)
DD(:,1)=P1;              % pressure
DD(:,3)=su1;             % su (cm/s)
DD(:,4)=Tu1;             % unburnt temperature (K)
DD(:,5)=k1;
end

% percentage and equivalence ratio
[NR,NC]=size(DD);
DD(NR+1:NR+2,1:5)=zeros(2,5);

    DD(NR+1,1)=Equiv;
    DD(NR+1,2)=Fco;
    DD(NR+1,3)=Fh2;
    DD(NR+1,4)=Fch4;
    DD(NR+1,5)=Fco2;

    DD(NR+2,1)=Fn2;
    DD(NR+2,2)=Fair;

fprintf('\n')
cd('d:\Multizone\Comparison\velocity');

[fname,newpath] = uiputfile('d:\Multizone\Comparison\velocity\*.csv','Choose Output File Name');
```

```
if findstr(fname,'csv')==isempty(fname)
  errordlg('filename should has csv','wrong file name');
end

file = fopen(fname,'w');  % creat a new file

% Write the data to the file
[n,m] = size(DD);
for i = 1:n
   for j = 1:m
      if j == m
         fprintf(file,'%5.6f,\n',DD(i,j));
      else
         fprintf(file,'%5.6f,',DD(i,j));
      end
   end
end

fclose(file);          % close the file
cd('d:\Multizone\Comparison')
```

Labview Data Acquisition Program:

The screen shots below shows the digital output for the spark ignition, and the subsequent data recording done by the labview program.